PB90-120064

Risk of Unsaturated/Saturated Transport and Transformation of Chemical Concentrations (RUSTIC). Volume 2. User's Guide

Woodward-Clyde Consultants, Oakland, CA

Prepared for:

Environmental Research Lab., Athens, GA

Jul 89

U.S. Department of Commerce
National Technical Information Service
NTIS

TECHNICAL REPORT DATA

(Please read Instructions on the reverse before completing)

1. REPORT NO.
EPA/600/3-89/048b

2.

3. RECIPIENT'S ACCESSION NO.
PB90 120064/AS

4. TITLE AND SUBTITLE
RISK OF UNSATURATED/SATURATED TRANSPORT AND TRANSFORMATION OF CHEMICAL CONCENTRATIONS (RUSTIC) Volume II: User's Guide

5. REPORT DATE
July 1989

6. PERFORMING ORGANIZATION CODE

7. AUTHOR(S)
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8. PERFORMING ORGANIZATION REPORT NO.

9. PERFORMING ORGANIZATION NAME AND ADDRESS
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[4]U.S. Environmental Protection Agency, Athens GA 30613

10. PROGRAM ELEMENT NO.
CCBE1A

11. CONTRACT/GRANT NO.
68-03-6304

12. SPONSORING AGENCY NAME AND ADDRESS
Environmental Research Laboratory - Athens, GA
Office of Research and Development
U.S. Environmental Protection Agency
Athens GA 30613

13. TYPE OF REPORT AND PERIOD COVERED

14. SPONSORING AGENCY CODE
EPA/600/01

15. SUPPLEMENTARY NOTES

16. ABSTRACT

The RUSTIC program links three subordinate models--PRZM, VADOFT, and SAFTMOD--in order to predict pesticide transport and transformation through the crop root zone, the unsaturated zone, and the saturated zone to drinking water wells. PRZM is a one-dimensional finite-difference model that accounts for pesticide fate in the crop root zone. This release of PRZM incorporates several features added to the original code--soil temperature simulation, volatilization and vapor phase transport in soils, irrigation simulation, and a method of characteristics algorithm to eliminate mumerical dispersion. PRZM now is capable of simulating the fate of the parent compound and up to two daughter species. VADOFT is a one-dimensional finite element code that solves the Richard's equation for flows in the unsaturated zone. The user may make use of constitutive relationships among pressure, water content, and hydraulic conductivity to solve the flow equations. VADOFT also may simulate the fate of two parent and two daughter products. SAFTMOD is a two-dimensional finite-element model that simulates saturated solute folw and transport in either an X-Y or X-Z configuration. The codes are linked with the aid of a flexible execution supervisor that allows the user to build models that are tailored to site-specific situations. To perform exposure assessments, the code is equipped with a Monte Carlo pre- and post-processor.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

18. DISTRIBUTION STATEMENT
RELEASE TO PUBLIC

19. SECURITY CLASS *(This Report)*
UNCLASSIFIED

20. SECURITY CLASS *(This page)*
UNCLASSIFIED

21. NO. OF PAGES
357

22. PRICE

United States
Environmental Protection
Agency

Environmental Research
Laboratory
Athens GA 30613

EPA/600/3-89/048b
July 1989

Research and Development

PB90-120064

EPA

Risk of Unsaturated/Saturated Transport and Transformation of Chemical Concentrations (RUSTIC)

Volume II: User's Guide

REPRODUCED BY
U.S. DEPARTMENT OF COMMERCE
NATIONAL TECHNICAL INFORMATION SERVICE
SPRINGFIELD, VA. 22161

EPA/600/3-89/048b

RISK OF UNSATURATED/SATURATED TRANSPORT AND TRANSFORMATION OF CHEMICAL CONCENTRATIONS (RUSTIC)

Volume II: User's Guide

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DISCLAIMER

The information in this document has been funded wholly or in part by the United States Environmental Protection Agency under Contract No. 68-03-6304 to Woodward-Clyde Consultants. It has been subject to the Agency's peer and administrative review, and it has been approved for publication as an EPA document. Mention of trade names of commercial products does not constitute endorsement or recommendation for use by the U.S. Environmental Protection Agency.

FOREWORD

As environmental controls become more costly to implement and the penalties of judgment errors become more severe, environmental quality management requires more efficient analytical tools based on greater knowledge of the environmental phenomena to be managed. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Assessment Branch develops management or engineering tools to help pollution control officials reach decisions on the registration and restriction of pesticides used for agricultural purposes.

The pesticide regulatory process requires that the potential risk to human health resulting from the introduction or continued use of these chemicals be evaluated. Recently much of this attention has been focused on exposure through leaching of pesticides to groundwater and subsequent ingestion of contaminated water. To provide a tool for evaluating this exposure, the RUSTIC model was developed. RUSTIC simulates the transport of field-applied pesticides in the crop root zone, the unsaturated zone, and the saturated zone to a drinking water well, taking into account the effects of agricultural management practices. The model further provides estimates of probable exposure concentrations by taking into account the variability in the natural systems and the uncertainties in system properties and processes.

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Director
Environmental Research Laboratory
Athens, Georgia

ABSTRACT

This publication contains documentation for the RUSTIC model. RUSTIC links three subordinate models in order to predict pesticide fate and transport through the crop root zone, unsaturated zone, and saturated zone to drinking water wells: PRZM, VADOFT, and SAFTMOD. PRZM is a one-dimensional finite-difference model which accounts for pesticide fate and transport in the crop root zone. This release of PRZM incorporates several features in addition to those simulated in the original PRZM code: specifically, soil temperature simulation, volatilization and vapor phase transport in soils, irrigation simulation and a method of characteristics (MOC) algorithm to eliminate numerical dispersion. PRZM is now capable of simulating fate and transport of the parent compound and up to two daughter species. VADOFT is a one-dimensional finite-element code which solves the Richard's equation for flows in the unsaturated zone. The user may make use of constitutive relationships between pressure, water content, and hydraulic conductivity to solve the flow equations. VADOFT may also simulate the fate and transport of two parent and two daughter products SAFTMOD is a two-dimensional finite-element model which simulates saturated solute flow and transport in either an X-Y or X-Z configuration. The codes are linked together with the aid of a flexible execution supervisor which allows the user to build models which are tailored to site-specific situations. In order to perform exposure assessments, the code is equipped with a Monte Carlo pre- and post-processor.

This report on the RUSTIC modeling system was submitted in fulfillment of two separate work assignments under Contract No. 68-03-6304 by Woodward-Clyde Consultants under the sponsorship of the U.S. Environmental Protection Agency. RUSTIC was developed by a Project Team headed by Woodward-Clyde Consultants as the prime contractor, with AQUA TERRA Consultants and HydroGeologic, Inc. as subcontractors. This report describes the work performed from January 1986 through September 1988. The final manuscript was prepared for publication and printing by AQUA TERRA Consultants under EPA Contract No. 68-03-3513.

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ACKNOWLEDGMENTS

A number of individuals contributed to this effort. Their roles are acknowledged in the following paragraphs.

Mr. Voos of Woodward-Clyde Consultants (WCC) programmed the execution supervisor and linked the models within the overall model architecture and design of RUSTIC developed by Mr. Jack Kittle of Aqua Terra Consultants. The model linkage was conceived by Mr. Dean and Dr. Atul Salhotra of WCC, Mr. Kittle, and Dr. Huyakorn. Dr. Huyakorn and his staff wrote the time/space bridging subroutines for the linkage.

Release II - PRZM was written by Dr. J. Lin and Mr. S. Raju of Aqua Terra Consultants under the direction of Mr. Donigian. Mr. Schanz (WCC) and Ms. Meeks (WCC) wrote the irrigation and MOC algorithms. Mr. Dean wrote the daughter products algorithms which were implemented by Dr. Lin.

The VADOFT code was written and documented by Dr. Huyakorn, H. White, J. Buckley, and T. Wadsworth of HydroGeologic. Mr. John Imhoff of Aqua Terra performed many useful testing simulations with VADOFT. SAFTMOD was written and documented by Dr. Huyakorn and J. Buckley.

The Monte Carlo pre- and post-processors were written by Dr. Salhotra, Mr. Phil Mineart, and Mr. Schanz of Woodward-Clyde. Final model assembly of the code and documentation and model testing was performed by Woodward-Clyde Consultants. Drs. Salhotra and P. Mangarella (WCC) peer reviewed the final documentation. The support of the editorial and graphics staff of WCC is appreciated.

The final manuscript was prepared for publication, incorporating review comments, by Ms. Susan Sharp-Hansen, Mr. S. Raju, and Ms. Dorothy Inahara of Aqua Terra Consultants.

The authors would like to acknowledge the support of the U.S. Environmental Protection Agency, and Mr. Lee Mulkey, Chief, Assessment Branch; Mr. Bob Carsel, Project Officer; and Dr. Rudy Parrish for their suggestions, input, and helpful comments.

SECTION 1

INTRODUCTION

This publication contains documentation for a linked model, known as RUSTIC, for contaminant transport in the root, vadose and saturated zones. A brief section on background and objectives for the model development effort follows in this introduction (Section 1.1). Section 1.2 gives a synopsis of risk and exposure assessment concepts. The reader who has sufficient background in these concepts may proceed to Section 1.3, which provides an overview of the RUSTIC linked modeling system, including major features and limitations. The documentation consists of two volumes, and Section 1.4 gives a synopsis of the contents of each. This introduction is common to both volumes.

1.1 BACKGROUND AND OBJECTIVES

The U.S. Environmental Protection Agency is continually faced with issues concerning the registration and restriction of pesticides used for agricultural purposes. Each of these regulatory processes requires that the potential risk to human health resulting from the introduction or continued use of these chemicals be evaluated. Recently, much of this attention has been focused on exposure through leaching of pesticides to groundwater and subsequent ingestion of contaminated water.

The capability to simulate the potential exposure to pesticides via this pathway has two major facets:

- Prediction of the fate of the chemical, after it is applied, as it is transported by water through the crop root zone, the vadose zone, and saturated zone to a drinking water well

- Evaluation of the probability of the occurrence of concentrations of various magnitudes at the drinking water well

There are a number of models which are capable of simulating the fate and transport of chemicals in the subsurface and in the root zone of agricultural crops. However, none of these models have been linked together in such a way that a complete simulation package, which takes into account the effects of agricultural management practices on fate and transport, is available for use either by the Agency or the agricultural chemical industry to address potential groundwater contamination problems. Without such a package, the decision maker must rely on modeling scenarios that are either incomplete or potentially incorrect. Each time a new scenario arises, recurring questions must be answered:

- What models should be used?
- How should mass transfer between models be handled?

The resolution of these issues for each scenario is both expensive and time consuming. Furthermore, it precludes consistency of approach to evaluation of contamination potential for various scenarios.

The modeling package described in this report seeks to overcome these problems by providing a consistent set of linked models which have the flexibility to handle a wide variety of hydrogeological, soils, climate, and pesticide scenarios. However, the formulation of the risk analysis problem requires more than a simple, deterministic evaluation of potential exposure concentrations. The inherent variability of force, capacitance and resistance in natural systems, combined with the inability to exactly describe these attributes of the system, suggests that exposure concentrations cannot be predicted with certainty. Therefore, the uncertainty associated with the predictions must be quantified. Consequently, this simulation package also seeks to provide this capability by utilizing Monte Carlo simulation techniques.

Stated more concisely, the objectives of this model development effort were to provide a simulation package which can:

- Simulate the fate and transport of field-applied pesticides in the crop root zone, the unsaturated zone, and the saturated zone to a drinking water well, taking into account the effects of agricultural management practices
- Provide probabilistic estimates of exposure concentrations by taking into account the variability in the natural systems and uncertainty in system properties and processes

Furthermore, it was desirable that the simulation package be easy to use and parameterize, and execute on the Agency's DEC/VAX machines. As a result, considerable effort has gone into providing parameter guidance for both deterministic and probabilistic applications of the model and software development for facile model implementation.

1.2 CONCEPT OF RISK AND EXPOSURE ASSESSMENT

Exposure assessment, as defined in the Federal Register (1984) for human impacts, is the estimation of the magnitude, frequency, and duration at which a quantity of a toxicant is available at certain exchange boundaries (i.e., lungs, gut, or skin) of a subject population over a specified time interval. Exposure assessment is an element of the larger problems of risk assessment and risk management, as demonstrated in Figure 1.1. The concentration estimates generated during an exposure assessment are combined with demographic and toxicological information to evaluate risk to a population--which can be used, in turn, to make policy decisions regarding the use or disposal of the chemical.

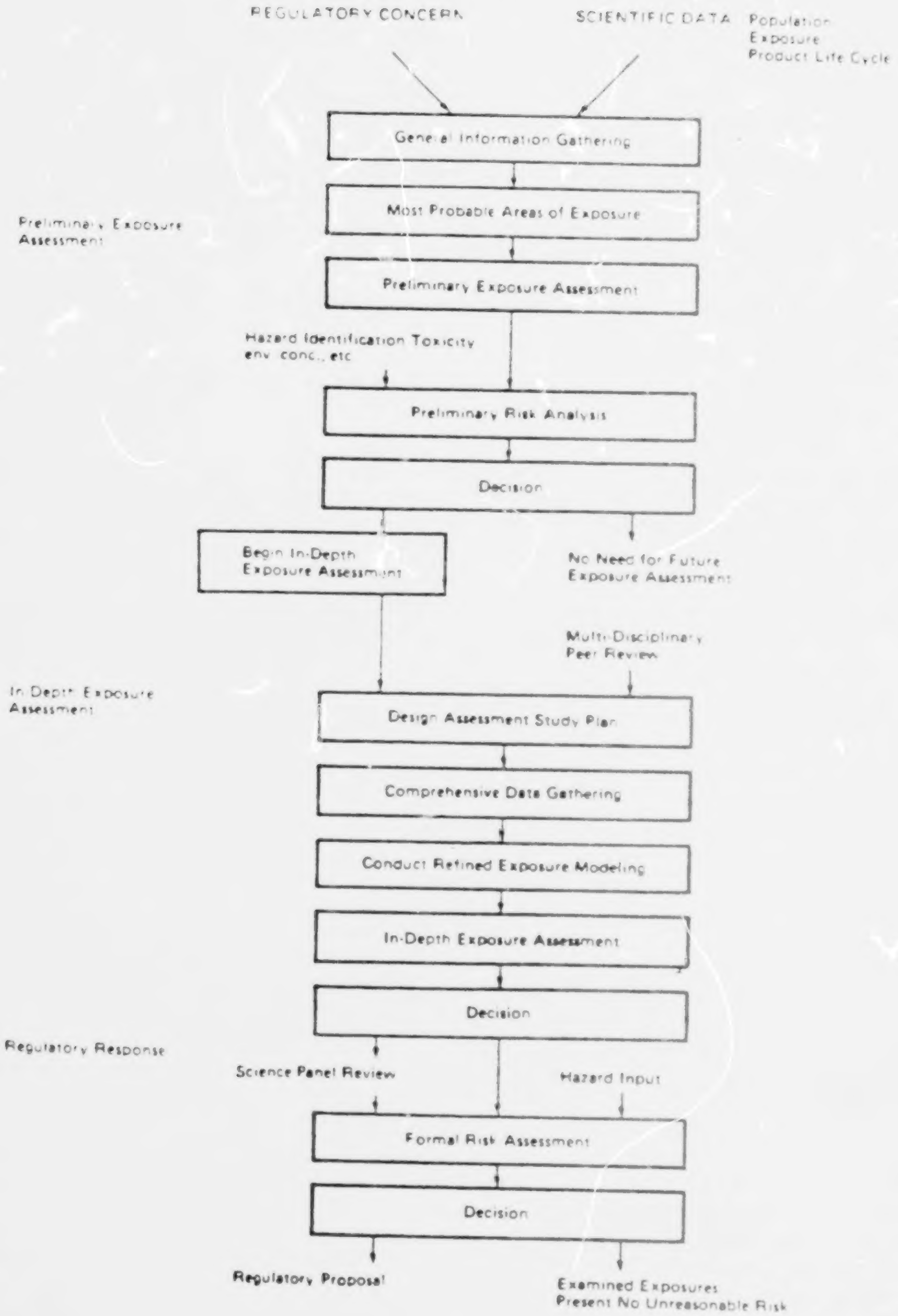

REGULATORY CONCERN
SCIENTIFIC DATA
Population
Exposure
Product Life Cycle
General Information Gathering
Most Probable Areas of Exposure
Preliminary Exposure Assessment
Preliminary Exposure Assessment
Hazard Identification Toxicity env. conc., etc
Preliminary Risk Analysis
Decision
Begin In-Depth Exposure Assessment
No Need for Future Exposure Assessment
Multi-Disciplinary Peer Review
In-Depth Exposure Assessment
Design Assessment Study Plan
Comprehensive Data Gathering
Conduct Refined Exposure Modeling
In-Depth Exposure Assessment
Decision
Regulatory Response
Science Panel Review
Hazard Input
Formal Risk Assessment
Decision
Regulatory Proposal
Examined Exposures Present No Unreasonable Risk

Figure 1.1. Decision path for risk assessment.

Major components of risk assessment are indicated below. Of these, the first three constitute the important steps for exposure assessment and are discussed in detail here.

- Characterization and quantification of chemical sources
- Identification of exposure routes
- Quantification of contaminant movement through the exposure routes to the receptor population/location
- Characterization of the exposed population
- Integration of quantified environmental concentrations with the characteristics of the exposed populations to yield exposure profiles

Characterization of sources(s) requires in a broad sense the estimation of the loading of a chemical into various environmental media. For the groundwater contamination problem, on a regional scale, this requires data on chemical uses and distribution of those uses (spatially and temporally). It also requires information on the crops being grown, registered or proposed chemical uses of those crops, and regional management practices. For a specific field-scale area, similar data would be needed to support an assessment; however, greater detail may be necessary.

The identification of exposure pathways involves a qualitative (or semiquantitative) assessment of how the chemical is thought to move from the source to the exposed population. Important fate processes which may serve to reduce the concentration of the chemical(s) along various pathways in different environmental media are also identified. For the case of groundwater exposure, important pathways and processes are predefined to a large extent in the models to be used.

The quantification of concentrations in a medium, given the source strength, pathways, and attenuation mechanisms along each pathway, is the next step, and is the major benefit of using models such as RUSTIC. The guidelines are very specific in the requirement that concentrations be characterized by duration and frequency as well as magnitude. These characteristics can be determined through the analysis of time series exposure data generated by the model.

The model produces a time series of toxicant concentrations in groundwater such as appears in Figure 1.2. The time series can be compared to a critical value of the concentration y. (This might be, for instance, the ADI [average daily intake level].) This type of analysis easily shows whether the criterion is exceeded and gives a qualitative feel for the severity of the exceedance state. A frequency distribution of the values of y (Figure 1.3) can be created by determining how often y is at a particular level or within a specific range. By choosing any value of y in Figure 1.2 and determining the area under the curve to the right of that value, Figure .4, which is a cumulative frequency distribution of the toxicant

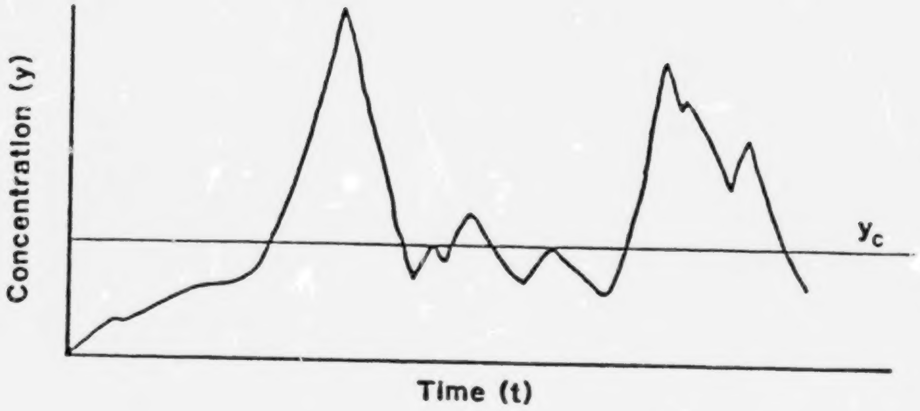


Figure 1.2. Time series plot of toxicant concentrations.

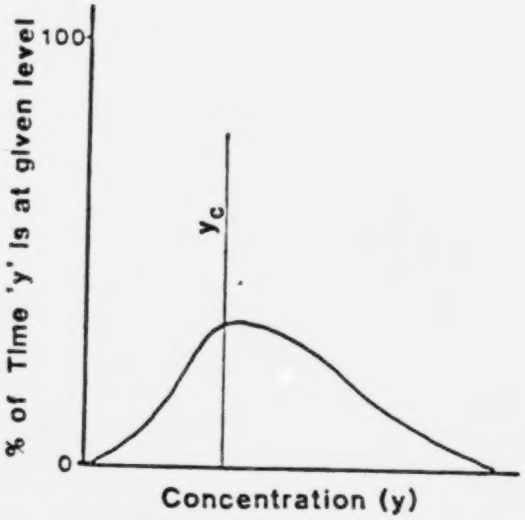


Figure 1.3.
Frequency distribution of toxicant concentrations.

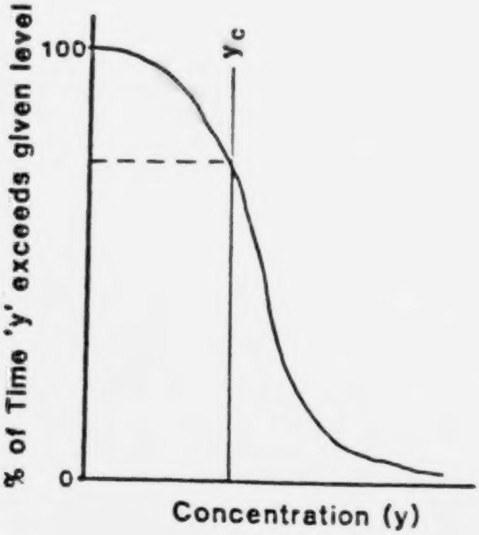


Figure 1.4.
Cumulative frequency distribution of toxicant concentrations.

concentration can be plotted. The cumulative frequency distribution shows the chance that any given value y will be exceeded. If the example time series is long enough, then the "chance" approaches the true "probability" that y will be exceeded.

Thus far, only the concentration to which the organism will be exposed has been discussed and nothing has been said concerning the duration of the event. If a window of length "t" is imposed on the time series at level y_c (Figure 1.5), and moved incrementally forward in time, a statement can be made concerning the toxicant concentration within the duration window. Normally, the average concentration within the window is used. The resulting cumulative frequency distribution shows the chance that the moving average of duration t_c will exceed the critical value of y, y_c. The moving average window should be the same length as that specified for y_c. For instance, in the case of cancer risk, a 70-year (lifetime) window is normally used to average the data in the simulated time series. The use of the moving window for averaging the time series allows us to compare both the concentration and duration against the standard. The chance or probability that the moving average concentration exceeds the standard is the essence of the exposure assessment. This type of information provides a precursor to the estimates of risk taken in using this chemical under the conditions of the model simulation. The use of models like RUSTIC which provide data of environmental concentrations and probability of occurrence ends here.

The next step in exposure assessment involves the characterization of the exposed population. Such factors as habits, age, sex, and location with respect to the source are of importance. The integration of concentration estimates and population characteristics makes possible the counting of the conditional events of concentration in an environmental medium and the

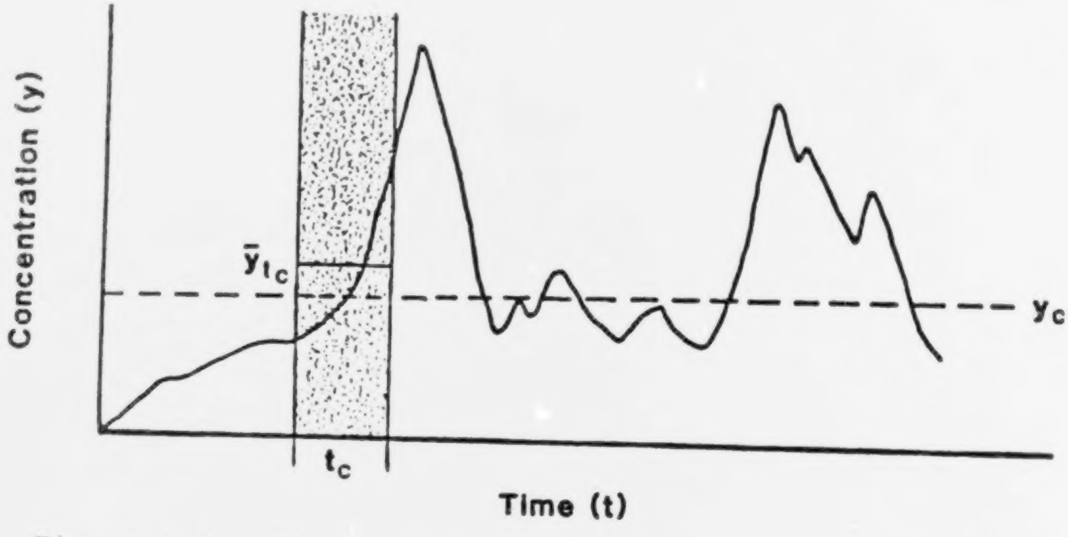


Figure 1.5. Time series of toxicant concentrations with moving average window of duration t_c.

opportunity for the population to be exposed to these concentrations. The exposure assessment ends at this point. The actual intake of chemicals, their fate within the human body (e.g., pharmacokinetics, toxicology), and their effects on the exposed population are not considered. These, however, are elements of the risk assessment.

Although the concepts underlying an exposure assessment are relatively simple, the actual application of these concepts is complicated because of large variations in source-specific and environment-specific characteristics and the necessity to integrate specialized knowledge from a number of different fields. This variability underscores the need to use a model such as RUSTIC in the evaluation of exposure concentrations.

1.3 OVERVIEW OF RUSTIC

This section gives an overview of the RUSTIC model highlighting the features and limitations of the simulation package as a whole and the component models PRZM, VADOFT, and SAFTMOD. The RUSTIC code was designed to provide state-of-the-art deterministic simulation of the fate and transport of pesticides, applied for agricultural purposes, in the crop root zone, the vadose zone, and the saturated zone. The model is capable of simulating multiple pesticides or parent/daughter relationships. The model is also capable of estimating probabilities of concentrations or fluxes in or fromthese various media for the purpose of performing exposure assessments.

To avoid writing an entirely new computer code, it was decided to make use of existing codes and software to the extent possible. Thus, due to its comprehensive treatment of important processes, its dynamic nature, and its widespread use and acceptability to the Agency and the agricultural chemical industry, the Pesticide Root Zone model (PRZM) (Carsel et al., 1984) was selected to simulate the crop root zone.

Having selected PRZM, several options were evaluated for developing the RUSTIC linked model to meet the objectives stated in Section 1.1. The first involved use of PRZM and a saturated zone model only. In this configuration, PRZM would be used to simulate both the root zone and the vadose zone. This option was eliminated because the assumptions of the elementary soil hydraulics in PRZM (i.e., drainage of the entire soil column to field capacity in one day) were considered inadequate for simulating flow in a thick vadose zone. The second involved the use of PRZM and a 2-D or 3-D variably saturated flow model. In this configuration, the latter model would represent both the vadose and saturated zones. Although the interface between the unsaturated and saturated zones would be more rigorously simulated, it was felt that the resulting code would be computationally too intensive for the intended application scenarios, and especially for use in a Monte Carlo (probabilistic) mode. Therefore, this option was also dropped.

The option finally selected is depicted in Figure 1.6. In this configuration, an enhanced version of PRZM is linked to a two-dimensional (single or two-layer) saturated zone model either directly or through a one-dimensional vadose zone flow and transport model. Both the vadose and saturated zone models simulate water flow and solute transport. A new code

(VADOFT) was written to perform the flow and transport simulation in the vadose zone, and an existing code was modified to produce the two-dimensional X-Y, X-Z or axisymmetric simulation model for the saturated zone (SAFTMOD).

A significant problem associated with this type of linkage is the difference in time scales of the individual models. While the vadose zone models are required to operate on a daily or less-than-daily time step, the time step of the saturated zone model could vary from days to months. A second problem is the correct interfacing of the vadose and saturated zone models, especially for the case of a fluctuating water table. This requires special handling of the spatial discretizations in the two models. The solution to these linkage problems is discussed in detail in Section 5.

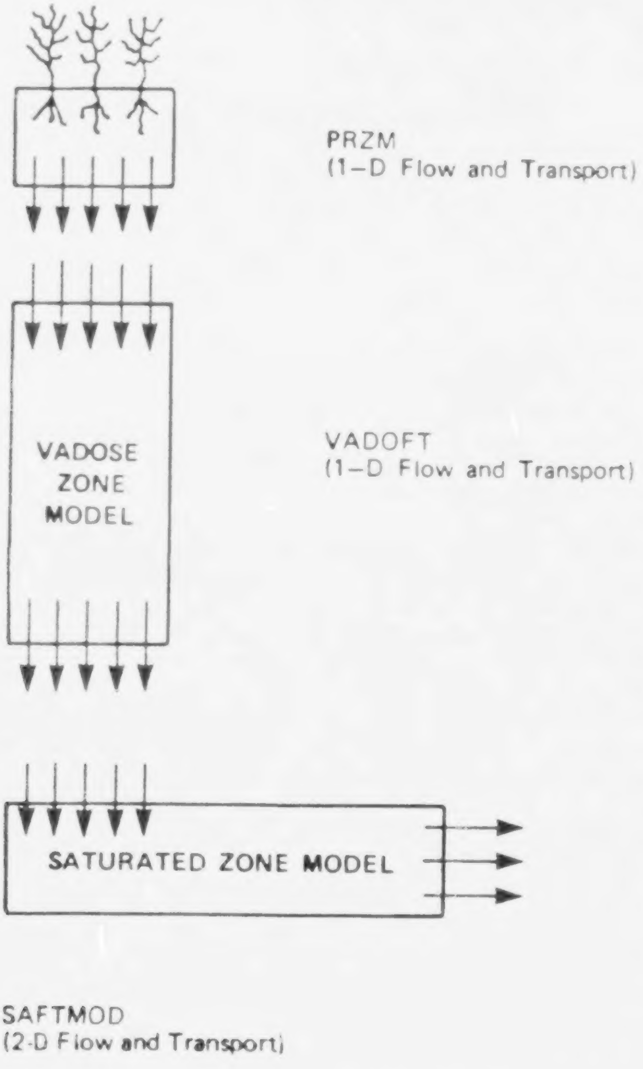

PRZM
(1-D Flow and Transport)
VADOSE
ZONE
MODEL
VADOFT
(1-D Flow and Transport)
SATURATED ZONE MODEL
SAFTMOD
(2-D Flow and Transport)

Figure 1.6. Linked modeling system configuration.

1.3.1 Overview of PRZM

1.3.1.1 Features--

The Pesticide Root Zone Model (PRZM) is a one-dimensional, dynamic, compartmental model that can be used to simulate chemical movement in unsaturated soil systems within and immediately below the plant root zone. It has two major components: hydrology (and hydraulics) and chemical transport. The hydrologic component for calculating runoff and erosion is based on the Soil Conservation Service curve number technique and the Universal Soil Loss Equation. Evapotranspiration is estimated either directly from pan evaporation data, or based on an empirical formula. Evapotranspiration is divided among evaporation from crop interception, evaporation from soil, and transpiration by the crop. Water movement is simulated by the use of generalized soil parameters, including field capacity, wilting point, and saturation water content. With a newly added feature, irrigation may also be considered.

The chemical transport component can simulate pesticide application on the soil or on the plant foliage. Dissolved, adsorbed, and vapor-phase concentrations in the soil are estimated by simultaneously considering the processes of pesticide uptake by plants, surface runoff, erosion, decay, volatilization, foliar washoff, advection, dispersion, and retardation. Two options are available to solve the transport equations: (1) the original backwards-difference implicit scheme that may be affected by excessive numerical dispersion at high Peclet numbers, or (2) the 'method of characteristics' algorithm which eliminates numerical dispersion while increasing model execution time.

Predictions are made on a daily basis. Output can be summarized for a daily, monthly, or annual period. Daily time series values of various fluxes or storages can be written to sequential files during program execution for subsequent analysis. In addition, a 'Special Action' option allows the user to output soil profile pesticide concentrations at user-specified times. With the Special Action option, the user can also change the values of certain parameters during the simulation period.

1.3.1.2 Limitations--

There were significant limitations in the original (Release I) version of PRZM. A few were obvious to the developers, while others were pointed out subsequently by model users. These are broken into four categories:

- Hydrology
- Soil hydraulics
- Method of solution of the transport equation
- Deterministic nature of the model

The Release II version of PRZM has been suitably modified to overcome many of these limitations.

Hydrologic and hydraulic computations are still performed in PRZM on a daily time step even though for some of the processes involved (evaporation, runoff, erosion) finer time step might be used to ensure greater accuracy and realism. For instance, simulation of erosion by runoff depends upon the peak runoff rate, which is in turn dependent upon the time base of the runoff hydrograph. This depends to some extent upon the duration of the precipitation event. PRZM retains its daily time step primarily due to the relative availability of daily versus shorter time step meteorological data. This limitation has in part been mitigated by enhanced parameter guidance.

In PRZM, Release I, the soil hydraulics were simple--all drainage to field capacity water content was assumed to occur within 1 day. (An option to make drainage time dependent was also included, but there is not much evidence to suggest that it was utilized by model users to any great extent.) This had the effect, especially in deeper soils, of inducing a greater-than-anticipated movement of chemical through the profile. While this representation of soil hydraulics has been retained in PRZM, the user has the option of coupling PRZM to VADOFT. PRZM is then used to represent the root zone, while VADOFT, with a more rigorous representation of unsaturated flow, is used to simulate the thicker vadose zone. The code VADOFT is discussed in more detail in a subsequent section. For short distances from soil surface to the water table, PRZM can be used to represent the entire vadose zone without invoking the use of VADOFT as long as no layers which would restrict drainage are present.

The addition of algorithms to simulate volatilization has brought into focus another limitation of the soil hydraulics representation. PRZM simulates only advective, downward movement of water and does not account for diffusive movement due to soil water gradients. This means that PRZM is unable to simulate the upward movement of water in response to gradients induced by evapotranspiration. This process has been identified by Jury et al. (1984) as an important one for simulating the effects of volatilization. However, the process would seem less likely to impact the movement of chemicals with high vapor pressures. For these chemicals, vapor diffusion would be a major process for renewing the chemical concentration in the surface soil.

Another limitation of the Release I model was the apparent inadequacy of the solution to the transport equation in advection-dominated systems. The backward difference formulation of the advection term tends to produce a high degree of numerical dispersion in such systems. This results in overprediction of downward movement due to smearing of the peak and subsequent overestimation of loadings to groundwater. In this new release, a new formulation is available for advection-dominated systems. The advective terms are decoupled from the rest of the transport equation and solved separately using the Method of Characteristics (MOC). The remainder of the transport equation is then solved as before, using the fully implicit scheme. This approach effectively eliminates numerical dispersion with, however, an increase in the computation time. In low-advection systems, the MOC approach reduces to the original PRZM solution scheme, which becomes exact as velocities approach zero.

The final limitation is the use of field-averaged water and chemical transport parameters to represent spatially heterogeneous soils. Several researchers have shown that this approach produces slower breakthrough times than are observed using stochastic approaches. This concern has been addressed by adding the capability to run PRZM in a Monte Carlo framework. Thus, distributional, rather than field-averaged, values can be utilized as inputs which will produce distributional outputs of the relevant variables (e.g., flux to the water table).

1.3.2 Overview of the Vadose Zone Flow and Transport Model (VADOFT)

VADOFT is a finite-element code for simulating moisture movement and solute transport in the vadose zone. It is the second part of the three-component RUSTIC model for predicting the movement of pesticides within and below the plant root zone and assessing subsequent groundwater contamination. The VADOFT code simulates one-dimensional, single-phase moisture and solute transport in unconfined, variably saturated porous media. Transport processes include hydrodynamic dispersion, advection, linear equilibrium sorption, and first-order decay. The code predicts infiltration or recharge rate and solute mass flux entering the saturated zone. Parent/daughter chemical relationships may be simulated. The following description of VADOFT is adapted from Huyakorn et al. (1988a).

1.3.2.1 Features--

The code employs the Galerkin finite-element technique to approximate the governing equations for flow and transport and allows for a wide range of nonlinear flow conditions. Boundary conditions of the variably saturated flow problems may be specified in terms of prescribed pressure head or prescribed volumetric water flux per unit area. Boundary conditions of the solute transport problem may be specified in terms of prescribed concentration or prescribed solute mass flux per unit area. All boundary conditions may be time dependent. An important feature of the algorithm is the use of constitutive relationships for soil water characteristic curves based on soil texture.

1.3.2.2 Limitations--

Major assumptions of the flow model are that the flow of the fluid phase is one-dimensional, isothermal and governed by Darcy's law and that the fluid is slightly compressible and homogeneous. Hysteresis effects in the constitutive relationships of relative permeability versus water saturation, and water saturation versus capillary pressure head, are assumed to be negligible.

Major assumptions of the solute transport model are that advection and dispersion are one-dimensional, and fluid properties are independent of contaminant concentrations. Diffusive/dispersive transport in the porous-medium system is governed by Fick's law. The hydrodynamic dispersion coefficient is defined as the sum of the coefficients of mechanical dispersion and molecular diffusion. Adsorption and decay of the solute is described by a linear equilibrium isotherm and a lumped first-order decay constant. Steady-state transport can not be simulated when decay is considered.

The code handles only single-phase flow (i.e., water) and ignores the presence of a second phase--i.e., air. The code does not take into account sorption nonlinearity or kinetic sorption effects which, in some instances, can be important. The code considers only single-porosity (granular) soil media. It does not simulate flow or transport in fractured porous media or structured soils.

1.3.3 Overview of the Saturated Zone Flow and Transport Model (SAFTMOD)

SAFTMOD is a finite element code for simulating groundwater flow and solute transport in the saturated zone. It is the third part of the three-component RUSTIC model for predicting the movement of pesticides within and below the plant root zone and assessing subsequent groundwater contamination. SAFTMOD performs two-dimensional simulations in an areal plane or a vertical cross section. In addition, the code can also perform axisymmetric simulations. Both single (unconfined or confined) and leaky two-aquifer systems can be handled. Transport of dissolved contaminants may also be simulated within the same domain. Transport processes accounted for include hydrodynamic dispersion, advection, linear equilibrium sorption, and first-order decay. Parent/daughter chemical relationships may be simulated. The following description of SAFTMOD is adapted from Huyakorn et al. (1988b).

1.3.3.1 Features--

The two dimensional analyses can be done in a transient or steady-state mode using SAFTMOD. The code employs the Galerkin finite-element technique to approximate the governing equations for flow and transport. For groundwater flow simulations the code accommodates water table conditions, recharge by infiltration or precipitation, and well pumping or injection. Boundary conditions of the saturated flow problem are specified in terms of prescribed hydraulic head (defined as the sum of pressure head and elevation), or prescribed volumetric water flux. Boundary conditions of the solute transport problem are specified in terms of prescribed concentration or prescribed solute mass flux. All boundary conditions can be time dependent.

1.3.3.2 Limitations--

The SAFTMOD code contains both saturated flow and solute transport models. Major assumptions of the flow model are that: Darcy's law is valid and hydraulic head gradients are the only significant driving mechanism for fluid flow, the porosity and hydraulic conductivity are constant with time, and gradients of fluid density, viscosity, and temperature do not affect the velocity distribution. For areal flow simulation in two-aquifer systems, vertical leakage is assumed in aquitards.

Major assumptions of the transport model are that fluid properties are independent of concentrations of contaminants. Contaminants are miscible with in-place fluids. For areal transport simulations, advection in aquitards is assumed to be negligible. Diffusive/dispersive transport in the porous medium system is governed by Fick's law. The hydrodynamic dispersion coefficient is defined as the sum of the coefficients of mechanical dispersion and molecular diffusion. Adsorption and decay of the solute may be described by a linear equilibrium isotherm and a first-order decay constant. Steady-state transport can not be simulated when decay is considered.

Other limitations of the SAFTMOD code are that it simulates only single-phase water flow and solute transport in saturated porous media. It does not consider unsaturated or fractured media. Non-Darcy flow that may occur near pumping wells is neglected. The code does not take into account sorption nonlinearity or kinetic sorption effects which, in some instances, can be important.

1.3.4 Model Linkage

One of the more challenging problems in this model development effort was the temporal and spatial linkage of the component models. In the section which follows, these linkages are discussed.

1.3.4.1 Temporal Model Linkage--

The resolution of the temporal aspects of the three models was straightforward. PRZM runs on a daily time step. The time step in VADOFT is dependent upon the properties of soils and the magnitude of the water flux introduced at the top of the column. In order for the nonlinear Richards' equation to converge, VADOFT may sometimes require time steps on the order of minutes. The SAFTMOD time step, on the other hand, would normally be much longer than one day.

For simplicity, it was decided that the time step of SAFTMOD would always be an integer multiple of PRZM's daily time step. This makes the direct linkage of PRZM to SAFTMOD in a temporal sense very straightforward. PRZM is simply run for the number of days of the SAFTMOD time step, SAFTMOD is then run, and so forth. The water and pesticide fluxes from PRZM are summed and averaged over the length of the SAFTMOD time step. SAFTMOD receives the time-averaged fluxes as input.

For the linkage of PRZM, through VADOFT, to SAFTMOD, the resolution of time scales is also straightforward. VADOFT is prescribed to simulate to a "marker" time value, specifically to the end of a day. The last computational time step taken by VADOFT is adjusted so that it coincides with the end of the day. PRZM's daily water fluxes are used as input to VADOFT. VADOFT utilizes this flux as a constant over the day and adjusts its internal computational time step in order to converge. PRZM and VADOFT execute for the number of days corresponding to the SAFTMOD time step. The output from VADOFT is then time averaged and used as input to SAFTMOD.

1.3.4.2 Spatial Linkages--

The spatial linkages utilized for the models are more complex. The principal problem is the presence of a fluctuating water table, which complicates the interfacing of the vadose (or root zone) and saturated zone codes. A second problem is that of the incompatibility between the hydraulics in PRZM and VADOFT. Of course, any linking scheme utilized must provide a realistic simulation of the flow of water and transport of solutes at the interfaces and must ensure mass balance.

PRZM and VADOFT--The major problem with the interfacing of these two models is that while VADOFT solves the Richards' equation for water flow in a variably saturated medium, PRZM uses simple "drainage rules" to move water through the soil profile. Because of this incompatibility, there may be times when PRZM produces too much water for VADOFT to accommodate within one day. This is very likely to happen in agricultural soils, where subsoils are typically of lower permeability than those of the root zone, which have been tilled and perforated by plant roots and soil biota. The result of this would be water ponded at the interface which would belong neither to PRZM or VADOFT.

The solution was to prescribe the flux from PRZM into VADOFT so that VADOFT accommodates all the water output by PRZM each day. This eliminates the problem of ponding at the interface. However, it does force more water into the vadose zone than might actually occur in a real system, given the same set of soil properties and meteorological conditions. The consequence is that water and solute are forced to move at higher velocities in the upper portions of the vadose zone. If the vadose zone is deep, then this condition probably has little impact on the solution. If it is shallow, however, it could overestimate loadings to groundwater, especially if chemical degradation rates are lower in the vadose zone than in the root zone.

VADOFT and SAFTMOD--The principal problem here is that of the presence of a dynamic boundary (rising and falling water table) between these models. Two approaches were considered to handle the problem. The first was to expand or contract the spatial domains of the models to accommodate the moving boundary. This is not a particularly insurmountable problem for the vadose zone model; however, for the saturated zone model it would require the addition of nodes at the upper boundary. This would require a constant evaluation and switching of the set of nodes receiving fluxes from the vadose zone. This appeared undesirable.

The second option was to overlap the spatial domains of the models and interpolate values for fluxes based upon the position of the water table. This latter approach was ultimately utilized. It has the additional feature of eliminating the effects of the bottom boundary conditions prescribed for the vadose zone model on the simulation of solute transport just above the water table. A detailed discussion of these spatial linkages is given in Section 5.

1.3.5 Monte Carlo Processor

RUSTIC can be run in a Monte Carlo mode so that probabilistic estimates of pesticide loadings to the saturated zone or concentrations in a well downgradient from the source area can be made. The input preprocessor allows the user to select distributions for key parameters from a variety of distributions; the Johnson family (which includes the normal and lognormal), uniform, exponential and empirical. If the user selects distributions from the Johnson family, he may also specify correlations between the input parameters. The Monte Carlo processor reads the standard deterministic input data sets for each model, then reads a Monte Carlo input file which specifies which parameters are to be allowed to vary, their distributions, the distribution parameters, and correlation matrix. The model then executes for a prespecified number of runs.

The output processor is capable of preparing statistics of the specified output variables including mean, maximum values and quantiles of the output distribution. The output processor also can tabulate cumulative frequency histograms of the output variables and send them to a line printer for plotting.

1.3.6 Overview Summary

A modeling system (RUSTIC) has been developed for the U.S. Environmental Protection Agency which is capable of simulating the fate and transport of pesticides, following application, through the crop root zone, vadose zone and saturated zone and into drinking water wells. The model is envisioned for use in simulating farms or small communities, and was designed to handle a variety of geometries likely to be encountered in performing evaluations for pesticide registration or special reviews. A major objective was also to keep the model simple and efficient, yet allow use in a Monte Carlo mode to generate probabilistic estimates of pesticide loadings or well water concentrations. The model consists of three major computational modules; PRZM, which performs fate and transport calculations for the crop root zone and is capable of incorporating the effects of management practices; VADOFT, which simulates one-dimensional flow and transport within the vadose zone; and SAFTMOD, which simulates two dimensional flow and transport in the saturated zone. SAFTMOD is capable of simulating a variety of aquifer geometries (water table, confined and leaky two-aquifer systems) and can perform areal, cross-sectional and axisymmetric simulations. Linkage of these models is accomplished through the use of simple bridging algorithms which conserve water and solute mass.

1.4 OVERVIEW OF VOLUMES I AND II

Documentation for RUSTIC has been produced in two volumes. The subject of Volume I is model theory and code verification or testing. It contains a description of the theory underlying the PRZM, VADOFT, and SAFTMOD codes. The description of each code includes a brief overview highlighting the features and limitations of each code. This is followed by detailed descriptions of the algorithms involved in each code and how they are solved numerically. The description of each of these models concludes with a section on algorithm testing. The fifth section of Volume I contains a description of the theory behind the linkage of the three codes to provide a cohesive simulation of the movement of pesticides following application, through the root zone, the vadose zone, and the saturated zone to a drinking water well. Section 6 of Volume I covers the theory behind the uncertainty preprocessor. Volume I concludes with model development references and appendices.

Volume II is a model user's guide. It opens with an introduction and a section on the installation of the code on the target computer systems. Section 3 has a user-directed overview of the model software, simulation modules, and a description of data bases for simulation support and parameter estimation. The fourth section takes the user through problem definition and model setup, and module input sequence building. Section 5 covers parameter estimation for the execution supervisor and each computational module. Section 6 takes the user through an example problem.

Following the references (Section 7), Section 8 contains appendices which include a listing of error messages and warnings, and a variable glossary.

SECTION 2

MODEL INSTALLATION AND EXECUTION

This section describes how to install the RUSTIC software on a computer, (including compilation and linking), how to verify that the software has been loaded correctly, and how to execute RUSTIC. The hardware and software required for installing RUSTIC are also discussed. As the program evolves over time, the installation and operational information described here is likely to change. If problems are experienced with this software, users should contact the EPA Center for Exposure Assessment Modeling (CEAM) at the Athens Environmental Research Laboratory in Athens, Georgia.

2.1 HARDWARE AND SOFTWARE REQUIREMENTS

RUSTIC development, testing, and maintenance at the EPA Athens Environmental Research Laboratory is performed on a Digital Equipment Corporation VAX machine running the VMS operating system. RUSTIC has also been successfully executed on a Prime 50 Series computer running PRIMOS, a Sun Microsystems 386i workstation (Unix/Sun OS), and an IBM-PC using a Definicon DSI-020 coprocessor board (with 2 MBytes of installed memory) and the MS-DOS operating system. The coprocessor board is required because of the large run-time memory requirements of the RUSTIC code. Although not yet tested, it should be possible to run RUSTIC on an IBM-PC compatible computer with 2-3 MBytes of memory, running under the OS/2 operating system, and using a FORTRAN compiler designed for OS/2 operation.

General hardware requirements for RUSTIC are 7 MBytes of available hard disk storage and 2-3 MBytes of available memory, depending on the specific computer and FORTRAN compiler being used. In addition, a 9-track tape drive or IBM-PC compatible 5.25 inch floppy disk drive (360 KB or 1.2MB) is required to download the software.

Software requirements are the operating system (listed above) and the standard FORTRAN 77 compiler and code linker for the target computer. Compilation of the code is necessary because the executable version (e.g EXE file) of a program is incompatible with other computer systems.

2.1.1 Software Requirements for IBM-PC/Definicon Systems

If the Definicon version of the RUSTIC code is being used, the program will be executed using the MS-DOS operating system. The RUSTIC software is compatible with the MS-DOS 3.21 and other versions which are able to recognize file directories. In addition, the Definicon Systems software loader must be available. The Definicon Systems documentation describes the modifications to the PATH statement necessary to accomplish this.

The DOS supplied ANSI.SYS driver must also be available. This driver is installed by modifying the DOS specific CONFIG.SYS file (located in the root directory) to contain the following line:

```
DEVICE = <path> ANSI.SYS
```

where <path> is the location (directory) of the ANSI.SYS file. This file will normally be located in a directory containing other DOS specific files.

The CONFIG.SYS file may have to be modified to specify how many files are available to the RUSTIC software. It the statement 'FILES =' is not present or it is present but with a value less than 20 (e.g., 'FILES = 10') then the statement 'FILES = 20' (without the quote marks) should be added to the CONFIG.SYS file.

If the installation disks are 360K Byte format, it will be necessary to have the DOS RESTORE command available. The RESTORE command is necessary since some files are larger than 360K and must be stored on more than one disk. The DOS RESTORE command (and the corresponding write utility, BACKUP) provide a convenient method to write and read files which are too large to fit on one disk.

2.2 RUSTIC INSTALLATION PROCEDURES

The installation procedures described in this section are intentionally general. Specific details will depend on the actual hardware, operating system, and file/directory structure of the target computer.

2.2.1 Copying the software to the hard disk

Transfer the software from tape or floppy disk to a new directory or subdirectory on the hard disk. The software consists of FORTRAN source code files (.FOR), FORTRAN 'include' files (.CMM .CMN .PRM .INC), and test input and output files. Depending on the computer and FORTRAN compiler, the FORTRAN source files may need to be renamed. The source code is distributed with .FOR suffixes, reflecting the VAX VMS FORTRAN compiler's standard name convention. Other compilers use the suffixes .F77 and .f to represent FORTRAN source code. Operating system commands using wild-card conventions for globally renaming similarly-named files should be utilized whenever they are available. For example, the DOS command for renaming all .FOR files to .F77 files is:

```
REN  *.FOR  *.F77.
```

2.2.2 Code modifications

As much as possible, the RUSTIC code has been designed to be implementation independent where an implementation would include computer make and type, input/output devices used, and brand and version of FORTRAN 77 compiler used. However, some incompatibilities may exist, particularly in the format of the

INCLUDE statement and file OPEN statements. In these cases, code modifications may be necessary, and should be made by someone having knowledge of FORTRAN programming on the target computer. Any text processor that operates on ASCII files without introducing control characters may be used to edit the source and/or 'include' files.

2.2.3 Compilation and linking

The FORTRAN source code must be compiled and linked using the existing FORTRAN compiler and code linker on the computer system. The 'include' files must be present in the same directory as the source files, and each source file must be compiled individually to produce a corresponding object file. For example, the VAX VMS command to compile a FORTRAN source file is: **FOR <filename>**, where <filename> is the name of the FORTRAN source code file, and the resulting object file has the suffix .OBJ.

The 'link' step combines the object files (produced in the compilation step) with standard library routines, and creates the executable program file. This process may be facilitated by a link 'command' file that lists all object files to be linked, specifies a name for the executable file, and other information needed by the linker software (e.g. the location of libraries to be searched for needed routines). The standard VAX VMS link command appropriate for RUSTIC is: **LINK RUSTIC.OBJ RUSTIC.OLB/LIB**, where RUSTIC.OBJ is the object file generated by compiling the 'main' program file (RUSTIC.FOR), and RUSTIC.OLB is the name of a library file containing all other RUSTIC object modules.

For VAX VMS systems, the command file RUSTBLD.COM is provided to perform both the compilation and link steps automatically. This file compiles all of the source files, stores the resulting object code in the library file RUSTIC.OLB, and links the program to produce the executable file RUSTIC.EXE.

2.2.4 Executing the test runs

The input and output files corresponding to two standard test runs are included in the RUSTIC software package to verify that the installation has been performed correctly. These tests are described in detail in Section 6 of this document, and general information regarding RUSTIC execution is included in Section 2.3 below. The RUSTIC run control input for these runs is contained in the files RUSTIC.RN1 AND RUSTIC.PN2, and the corresponding output files have the suffixes .VF1 and VF2. Since the program requires the run control input file to be named RUSTIC.RUN, the test runs can be executed individually by: (1) copying the appropriate test input file to a new file with the name RUSTIC.RUN, (2) erasing any output files from a previous run, if present, and (3) typing RUSTIC (followed by a return) to start execution.

During execution of the test runs, RUSTIC creates an output file named KECHO.PRN, and several component model output files with the suffix or extension .PRn, where n is 1 or 2. The KECHO.PRN file (for each run) and each of the PRn output files should be compared to the corresponding VFn output file, supplied for verification of the code, either by using an editor to visually compare the results, or by using a compare utility such as

DIFFERENCES on a VAX VMS computer or COMP or FC on DOS computers. If the PRn files do not match the VFn files, some aspect of the installation may be incorrect. Small differences in the values of floating point output may occur normally between different computer hardware/software systems; therefore, depending on the magnitude of the differences, a decision can be made to consult with EPA CEAM personnel at the Athens ERL to determine the source of the problem. The VFn files distributed with the software were generated using a VAX VMS system, so very few or no differences should be observed on VAX computers.

2.3 GENERAL PROCEDURES FOR RUSTIC EXECUTION

This section contains descriptions of techniques and suggestions for normal (operational) execution of RUSTIC. It is generally convenient to locate all of the input files pertaining to a specific problem within their own subdirectory. The input files should be developed using the file descriptions of Section 4.2. It will normally be useful to start with the test input data files provided and edit them to meet the specifications of the problem at hand.

The names chosen for the input files should be specific to the problem to reduce the potential for confusing these files with those developed for alternate problems -- RUSTIC enforces no restrictions on the names chosen, either for the prefix or extension (the operating system used may, however, enforce restrictions; e.g., MS-DOS limits the prefix to 8 characters and the extension to 3 characters). The file name length, including the path, must be less than 81 characters. It is good practice to choose an extension which implies an input file (e.g., .IN or .DAT) or output file (e.g., .OUT or .PRN). The names of the files used and the path describing where the files are located (the subdirectory) are defined in the file RUSTIC.RUN, the run control file (see Section 4.2.1). The file RUSTIC.RUN must be in the subdirectory from which the execution is initiated. When all of the necessary files are complete, RUSTIC can be executed by typing RUSTIC followed by a return.

The PATH statement in the RUSTIC.RUN file can be used to specify the directories or subdirectories where the model input and output files are located. When the PATH statement is used in the RUSTIC.RUN file, the defined path must include all necessary characters such that, when inserted in front of the file name, a complete path + file name string is formed. For the MS-DOS operating system, this implies that the path must end with the backslash character ('\'). The defined path will pertain to all files which are defined after that path statement until another path is defined.

The path record can also be used to define files which are located on different drives. This is potentially useful to increase execution speed. Scratch (unformatted) files are used by PRZM, VADOFT, and SAFTMOD for temporary storage of data and these scratch files are opened with the last defined path. If the last path indicates that the files are to be located on a RAM disk (if a RAM disk is available with the operating system used), execution speed will be measurably increased.

Input files are opened with STATUS = 'OLD', which means that they must exist (in the directory specified) for the software to continue the current simulation. If the specified file does not exist, a fatal error is issued and the simulation is terminated.

Output files are opened with STATUS = 'NEW'. Different FORTRAN compiler/ operating systems have different responses to opening a file with STATUS = 'NEW' when the file is present. Some will ignore the file's presence and overwrite it. Others will issue a fatal error and the simulation will be terminated. If this is the case, the user will have to ensure that the names chosen for output files of the current simulation do not correspond to existing file names.

In addition to file opening errors, the RUSTIC code checks for errors within the input files and internal (calculation) errors. A complete list of the error messages provided for error conditions currently recognized by the code is provided in Appendix 8.1.

A screen management routine has been supplied to display the software in operation. This routine lists RUSTIC execution information (line-by-line) to the standard output device. Note that the echo level and trace level (see Section 4.2.1) can be used to increase or decrease the amount of information being sent to the screen.

SECTION 3

MODULES AND LOGISTICS

The RUSTIC model consists of six major modules. These are:

- EXESUP, which controls the simulation
- IMPREA, which performs data input and initialization functions and echoes input to an output file
- PRZM, which performs fate and transport computations for the crop root zone
- VADOFT, which performs fate and transport computations for the vadose zone
- SAFTMOD, which performs fate and transport calculations for the saturated zone
- MCARLO, which performs functions related to Monte Carlo simulation

These components combine to allow the user to simulate the fate and transport of agriculturally applied chemicals through the root zone, vadose zone, and saturated zones, and to determine the magnitude of the resulting concentrations in drinking water wells. Some special features that the model possesses are the capability of PRZM to simulate volatilization and vapor phase movement of chemical, irrigation effects on pesticide leaching and the capability of each of the modules to simulate the formation, fate, and transport of daughter products. SAFTMOD has the capacity to simulate a variety of aquifer configurations. In the following sections, the functions and capabilities of each of these modules are discussed more fully.

3.1 EXESUP - THE EXECUTION SUPERVISOR

The execution supervisor controls the simulation. It opens files, reads in and initializes data (by calling INPREA), controls the "networking" of computational modules, controls any Monte Carlo simulation, and eventually closes files and terminates the simulation. The execution supervisor has its own input file, the contents of which are detailed in Section 4.2.1. In order to set up this input file, the user must have planned out the module networking and system configuration, starting and ending simulation dates, and other data to control the simulation and model output.

3.2 PRZM - THE ROOT ZONE FATE AND TRANSPORT MODULE

PRZM performs computations of fate and transport in the crop root zone. To do this, it requires soils, pesticides, crop, meteorology, and agronomic practice input data. PRZM input data are discussed in Section 4.2.2.

In order to use PRZM, two files are required. The first is a meteorologic file which contains precipitation, temperature, pan evaporation, wind speed, and solar radiation data. Some meteorologic data files available to aid the user in applying PRZM or RUSTIC are described in Section 3.8. The second file required is the PRZM parameter file. Guidance for estimating PRZM parameters is given in Section 5.2.

In the framework of the linked modeling system, the major outputs of PRZM are the time series of water and chemical flux to the vadose zone, or saturated zone, depending upon how the network is defined by the user. PRZM, however, produces two individual output files:

1) A summary file containing:

- A hydrologic summary (daily, monthly, or annual)
- A pesticide mass summary (daily, monthly, or annual)
- A pesticide concentration summary (daily, monthly, or annual)

2) A time series file which writes out daily values of the requested variables as either a time series or cumulative time series

3.2.1 Special Actions Option

The Special Actions option in PRZM allows the user to output soil profile pesticide concentrations at user-specified times during the simulation period, and to change selected model parameters to better represent chemical behavior and the impacts of agricultural management practices. The required input format and parameters are specified in Volume II, Section 4.

By using the 'SNAPSHOT' capability of Special Actions, the user can output the pesticide concentration profile, i.e., the total concentration in each soil compartment, for any user-specified day during the simulation period. In this way, the user can run PRZM with only monthly or annual output summaries and still obtain simulation results for selected days when field data were collected. There is no inherent limit to the number of SNAPSHOTs that can be requested in a single run. When more than one chemical is being simulated, the concentration profiles are provided by the order of the chemical number, i.e., NCHEM.

To better represent the expected behavior of the chemical being simulated, or the impacts of tillage or other agricultural practices, the following parameters can be reset to new values at any time during the simulation period:

Solution Decay Rate (DWRATE)
Sorbed Decay Rate (DSRATE)
Partition Coefficient (KD)

Bulk Density (BD)
Curve Number (CN)
USLE Cover Factor (USLEC)

Thus, for chemicals that demonstrate seasonal decay rates or partition coefficients, or different values for the period following application compared to later in the crop season, the appropriate parameters can be changed at user-specified times to mimic the observed, or expected, behavior of the compound.

Similarly, for agricultural practices or specific tillage operations that impact the soil bulk density, curve number, or cover factor, these parameter values can be altered during the simulation in an attempt to better represent their impacts. The parameter guidance provided in Volume II, Section 5.2, may help the user in determining adjustments for these parameters. Users should note that adjustments to the bulk density, and possibly the partition coefficient, may impact the pesticide balance calculation.

3.3 VADOFT - THE VADOSE ZONE FATE AND TRANSPORT MODULE

VADOFT performs computations of fate and transport in the vadose or unsaturated zone. In order to do this, it requires soil, soil-water, and chemical specific information. It also requires initial (water and chemical) conditions and boundary conditions. Input data file building is discussed in Section 4.2.2 and parameter estimation guidance is given in Section 5.3. In the linked system, it obtains its upper boundary conditions from PRZM output (i.e., root zone water and chemical fluxes). Note that if VADOFT is run in tandem with PRZM, then VADOFT always uses a prescribed water flux at the upper boundary and a prescribed head at the lower boundary node for flow simulation and a prescribed mass flux at the upper boundary node and zero concentration condition at the lower boundary node for transport simulation. If SAFTMOD is being run, it obtains an updated lower boundary condition (hydraulic head) based on SAFTMOD flow results after each executed SAFTMOD timestep. Unlike PRZM, which performs flow and transport computations in a single "pass", VADOFT may be used to solve either flow or transport problems individually. Because of this, VADOFT must be called twice in the linked model (once for flow, once for transport) for each day of transport simulation. A scratch file is used to save flow information (velocities, etc.) in order to perform a transport simulation. For guidance on the required scratch file, please refer to Section 4.2.1.

Another consideration for the use of VADOFT is that it solves a set of non-linear equations for flow, and hence an iterative solution is required. This has the dubious distinction of making the flow portions of VADOFT one of the slower portions of the code to execute and introduces the possibility of model failure due to nonconvergence. With judicious parameter selection, the latter can be avoided.

In the context of the linked modeling system, the most important VADOFT outputs are the water and mass fluxes to user-designated SAFTMOD nodes. Of course, the model produces various outputs. The primary line printer output from the flow model of VADOFT includes nodal values (at various time steps) of pressure head and nodal values of vertical Darcy velocity and saturation at various time steps. The frequency of printing of the flow and transport results is controlled by the frequency of printing of PRZM hydrology and pesticide summaries.

3.4 SAFTMOD - THE SATURATED ZONE FATE AND TRANSPORT MODULE

SAFTMOD performs chemical fate and transport computations in the saturated zone. Like VADOFT, it requires data on aquifer materials, chemical properties, and initial and boundary conditions. Some of the network information for PRZM or VADOFT linkage to SAFTMOD is also input in its parameter file. Boundary conditions (i.e., water and mass fluxes) are provided by VADOFT or PRZM when the model is run as part of the linked system.

Like VADOFT, SAFTMOD solves either a flow or transport problem and uses scratch files to store parameters and initial conditions to restart flow or transport simulations. It uses a scratch file, like VADOFT, to store information (velocities, etc.) for a transport simulation from a corresponding flow simulation. Guidance for setting up the scratch file is found in Section 4.2.1.

In a typical application of the linked modeling system, the SAFTMOD output of greatest interest would be the time series of pesticide concentrations in the drinking water well or at a specific location in the aquifer. Other outputs (e.g., head or concentration maps) may be useful for calibration purposes. The primary line printer output from the flow model of SAFTMOD includes model values (at various time levels) of hydraulic head and nodal values of Darcy velocity components at various time steps. The primary line printer output of the transport model of SAFTMOD includes nodal values (at various time levels) of solute concentration. When run in the linked nodes. SAFTMOD like VADOFT, keys off the printing frequency of PRZM (daily, monthly, or annual).

3.5 MCARLO - THE MONTE CARLO SIMULATION MODULE

MCARLO performs all the functions necessary to execute a Monte Carlo simulation. It reads special data for parameters to be varied (e.g., distribution types and moments) and output variables to be observed, generates random numbers, correlates them and performs transformations, exchanges these generated values for RUSTIC parameters, performs statistical analysis on the output variables, and writes out statistical summaries for the output variables.

The MCARLO module makes use of an input and output file. Inputs to the MCARLO module are discussed in Section 4.2.5. The user should be aware that any of the parameters entered in the Monte Carlo input file once designated as constants will be used in lieu of that same parameter value entered in the standard input file.

3.6 MODEL STRUCTURE

This section discusses model structure. Specifically, it gives information on model modules and subroutines and module communication.

3.6.1 Subroutine Descriptions

As discussed above, RUSTIC is organized into a number of modules, each having subroutines which perform various specific functions. In this section, Table 3-1 gives a listing of all the major subroutines called by the program. Subroutines are organized alphabetically by module or calling subroutine. A brief description of the function of each subroutine is also given.

A glossary of the major internal variable names used within the RUSTIC code is provided in Appendix 8.2.

3.6.2 Intra/Intermodule Communication

Communication between subroutines and modules utilizes common blocks and argument lists. The primary modes of data transfer are via common blocks. Common blocks utilized in the program are listed in Table 3-2 along with a brief topical description of their contents.

Subroutine arguments are used to transfer some data within the program. This method is primarily used where common blocks are infeasible and to isolate variables in certain sections of the code which may have the same name. For instance, the array DIS is used in both VADOFT and SAFTMOD as the storage array for head and concentration values. Subroutine arguments are used to pass values of DIS from VADOFT and SAFTMOD into the execution supervisor (EXESUP) in which both of these arrays must be known.

Dimensions of most program arrays are specified in PARAMETER statements. The variables used to size program arrays are listed in Table 3-3 along with a description and default value. The user should select values for these variables based upon the array sizes necessary to simulate the problem of interest.

3.7 LIMITATIONS

The user should be aware of several limitations of the code as it is currently implemented. Originally, the intent was to allow for multiple applications of the PRZM and VADOFT codes to simulate large scale lateral heterogeneities in a physical system. Although a perusal of the code will show that there is a substantial amount of logic built in to accommodate this feature, it has not yet been fully implemented.

The second limitation is that, in the current version, daughter products cannot be simulated in either aquitards or a multiaquifer system. There, the simulation of daughter products is limited to PRZM, VADOFT, and a single water table aquifer system.

The final limitation is that only a small number of input variables may be changed at random by invoking the Monte Carlo routines. It is not difficult to add additional variables, however.

Table 3-1. LIST OF SUBROUTINES BY MODULE AND A DESCRIPTION OF THEIR FUNCTIONS

Module/ Calling Subroutine	Subroutine	Function
RUSTIC	CLOSIT	Closes all files prior to program termination.
	DISPLY	Displays a message on the screen and on the output echo file.
	DONBAR	Tracks the "Percentage Completion" of the simulation.
	EXESUP	Execution supervisor. Calls computational modules and linkage routines.
	INITEM	Determines user defined options, opens files, and reads global data.
	INITMC	Initializes Monte Carlo parameters.
	INPREA	Driver subroutines for reading and initializing program input data.
	OUTPUT	Generates Monte Carlo output.
	RANDOM	Generates random numbers for Monte Carlo simulations.
	READM	Reads user defined Monte Carlo variables.
	SCREEN	Screen manager routine.
	STATIS	Calculates statistical summaries of Monte Carlo output variables.
EXESUP	DISPLY	See "RUSTIC".
	DONBAR	See "RUSTIC".
	ENDDAY	Calculates the last day of the current simulation period.
	GLOMAS	Performs global mass balance for the linked system.
	SMIOIN	Reads SAFTMOD input file.
	SUBIN	Tracks entries into subroutines.

Table 3-1. LIST OF SUBROUTINES BY MODULE AND A DESCRIPTION OF THEIR FUNCTIONS (continued)

Module/ Calling Subroutine	Subroutine	Function
	SUBOUT	Tracks exits from subroutines.
	XFLOW	Calls VADOFT and/or SAFTMOD for flow simulations.
	XPRZM	Calls PRZM module and stores intermediate results for linkage with VADOFT and SAFTMOD.
	XTRANS	Calls VADOFT and/or SAFTMOD for transport simulations.
	ZONEAV	Calculates zonal average values of water table elevations/pressure heads.
INITEM	ADDSTR	Adds a character string to another character string.
	BMPCHR	Capitalizes a character string.
	CHKFIL	Checks "Open" status of a file.
	CLOZE1	Closes one file.
	COMRD	Allows user to insert comments in data files by ignoring comments when reading.
	COMRD2	Comment reading routine which handles end-of-file read.
	ECHOGD	Echoes global data input.
	ECHOF	Echoes the names of files opened.
	ELPSE	Printing utility.
	ERRCHK	Writes error messages, closes files if fatal error.
	LFTJUS	Left justifies a character string.
	NAMFIX	Left justifies and capitalizes a character string.
	OPECHO	Printing utility.
	OPENF	Opens files.

Table 3-1. LIST OF SUBROUTINES BY MODULE AND A DESCRIPTION OF THEIR FUNCTIONS (continued)

Module/ Calling Subroutine	Subroutine	Function
	PRZDAY	Transfers simulation start and end dates to PRZM common.
	SCREEN	See "RUSTIC".
	TDCALC	Calculates total number of days in a simulation.
	VALDAT	Checks user supplied date for validity.
INPREA	CLOZE1	See "INITEM"
	ECHO	Echoes PRZM input file read.
	ERRCHK	See "INITEM"
	INIACC	Initializes PRZM accumulators.
	INITL	Initializes PRZM variables.
	MCPRZ	Transfers random values to PRZM variables for Monte Carlo simulations.
	PRZMRD	Reads PRZM input file.
	RSTPT1	Stores PRZM initial conditions on unformatted file.
	RSTPUT	Stores PRZM initial conditions on unformatted file.
	SCREEN	See "RUSTIC".
	SMIOIN	See "EXESUP".
	SUBIN	See "EXESUP".
	SUBOUT	See "EXESUP".
	VADINP	Reads VADOFT input sequence.
XPRZM	DISPLY	See "RUSTIC".
	PRZM	Performs root zone fate and transport calculations.
	SUBIN	See "EXESUP".

Table 3-1. LIST OF SUBROUTINES BY MODULE AND A DESCRIPTION OF THEIR FUNCTIONS (continued)

Module/ Calling Subroutine	Subroutine	Function
	SUBOUT	See "EXESUP".
XFLOW	DISPLY	See "RUSTIC".
	LINTRP	Interpolates daily values of the water table elevation (Function 1) and interpolates daily values of pesticides flux using PRZM/VADOFT normal fluxes to estimate flux to the water table.
	MCSFT	Transfers Monte Carlo simulation variables to SAFTMOD arrays.
	MCVAD	Transfers Monte Carlo simulation variables to VADOFT commons.
	SCREEN	See "RUSTIC".
	SFTMOD	Performs saturated zone fate and transport calculations.
	SMIOIN	See "EXESUP".
	SUBIN	See "EXESUP".
	SUBOUT	See "EXESUP".
	SWFLX	Loads water fluxes from PRZM/VADOFT into SAFTMOD arrays.
	VADINP	See "INPREA".
	VADOFT	Performs vadose zone fate and transport calculations.
	WMFCAL	Integrates daily PRZM/VADOFT fluxes to pass into SAFTMOD.
	ZONEAV	See "EXESUP".
XTRANS	DISPLY	See "RUSTIC".
	INITDK	Initializes VADOFT chemical array.

Table 3-1. LIST OF SUBROUTINES BY MODULE AND A DESCRIPTION OF THEIR FUNCTIONS (continued)

Module/ Calling Subroutine	Subroutine	Function
	LINTRP	See "XFLOW".
	MASCOR	Corrects nodal concentrations of PRZM/VADOFT nodes beneath the water table based on SAFTMOD simulation results.
	MCSFT	Transfers SFTMOD output to Monte Carlo variables.
	MCVAD	Transfers VADOFT output to Monte Carlo variables.
	SFTCHM	Loads chemical specific data into SAFTMOD arrays.
	SFTFLX	Loads PRZM/VADOFT mass fluxes into SAFTMOD arrays.
	SFTMOD	See "XFLOW"
	SMIOIN	See "EXESUP".
	SUBIN	See "EXESUP".
	SWFLX	See "XFLOW".
	VADINP	See "INPREA".
	VADCHM	Loads chemical specific data into VADOFT arrays.
	VADOFT	See "XFLOW".
	WMFCAL	See "XFLOW".
PRZM	ACTION	Identifies and performs special action.
	BLOCK DATA	Initializes CNDMO, CMONTH and CDATE values for common block MISC.
	CANOPY	Calculates the vertical transport resistances of plant canopy.
	EROSN	Computes loss of pesticide due to erosion.
	EVPOTR	Computes daily potential evapotranspiration, canopy evaporation and actual evapotranspiration from soil layers.

Table 3-1. LIST OF SUBROUTINES BY MODULE AND A DESCRIPTION OF THEIR FUNCTIONS (continued)

Module/ Calling Subroutine	Subroutine	Function
	FTIME	Stores current time and date (for PDP 11/70 only).
	FURROW	Computes flow and infiltration down a furrow using a kinematic wave with Green-Ampt infiltration.
	HYDROL	Performs hydrologic calculations for snowmelt, crop interception, runoff and infiltration.
	HYDR1	Performs hydraulic calculations for soil under free drainage conditions.
	HYDR2	Performs hydraulic calculations for soil under restricted drainage conditions.
	INFIL	Computes Green-Ampt infiltration assuming a constant depth over time step DT.
	IRRIG	Determines soil moisture deficit, decides if irrigation is needed, and calculates irrigation depths.
	KDCALC	Calculates K_d values based on (1) Karickhoff (2) Kenaga or (3) Chiou method.
	KHCORR	Corrects temperature effect on Henry's constant.
	MASBAL	Calculates mass balance error terms for both hydrology and pesticide transport.
	MOC	Computes pesticide transport due to advective influence.
	OUTCNC	Prints daily, monthly or annual pesticide concentration profiles.
	OUTHYD	Accumulates and outputs daily, monthly or annual summaries for water.
	OUTIRR	Outputs irrigation results.
	OUTPST	Accumulates and outputs daily, monthly or annual summaries for pesticides.

Table 3-1. LIST OF SUBROUTINES BY MODULE AND A DESCRIPTION OF THEIR FUNCTIONS (continued)

Module/ Calling Subroutine	Subroutine	Function
	OUTRPT	Prints daily, monthly and annual pesticide concentration profiles to MODOUT and SNAPSHOT output files.
	OUTTSR	Outputs user specified time series to time series plotting files.
	PESTAP	Computes amount and location of pesticide application (foliage, soil surface, soil incorporated).
	PLGROW	Determines plant growth parameters.
	PLPEST	Computes loss of pesticide in plant canopy compartment.
	PSTLNK	Provides linkage for transformation and source terms for parent/daughter relationships.
	SLPST0	Sets up the coefficient matrix for the solution of the soil pesticide transport equation considering advection (implicit backwards difference formation).
	SLPST1	Sets up the coefficient matrix for the solution of the soil pesticide transport equation without considering advection (MOC formulation).
	SLTEMP	Calculates soil temperature profile.
	THCALC	Computes field capacity and wilting point for each soil layer.
	TRDIAG	Solves a system of equations with a tridiagonal coefficient matrix in double precision.
	TRDIA1	Solves a system of equations with a tridiagonal coefficient matrix in single precision.
VADOFT	ASSEMF	Computes and assembles element matrices for variably saturated water flow simulation.

Table 3-1. LIST OF SUBROUTINES BY MODULE AND A DESCRIPTION OF THEIR FUNCTIONS (continued)

Module/ Calling Subroutine	Subroutine	Function
	ASSEMT	Computes and assembles element matrices for solute transport simulation.
	BALCHK	Performs mass balance computation and computes total solute mass flux at each node.
	CONVER	Determines limiting value of water saturation that will be used in the subsequent computation.
	DSWFUN	Computes moisture capacity function.
	HFINTP	Determines the prescribed head or flux values by interpolation.
	INTERP	Performs linear interpolation using tabulated data of relative permeability versus water saturation, and pressure head versus water saturation.
	PKWFUN	Computes relative permeability function.
	SWFUN	Computes water saturation function.
	TRIDIV	Performs tri-diagonal matrix solution.
	VARCAL	Computes current nodal values of head or concentration.
	VSWCOM	Computes nodal values of water saturation and Darcy velocity.
SFTMOD	ANDCAL	Computes nodal lengths and areas.
	ASSEMV	Assembles element matrices and right-hand-side vector into global coefficient matrix and global right-hand-side vector. Also incorporates nonzero flux boundary conditions into the global right-hand-side vector.
	BALCHS	Performs the mass balance computation.
	BUPDAT	Updates boundary conditions arrays.

Table 3-1. LIST OF SUBROUTINES BY MODULE AND A DESCRIPTION OF THEIR FUNCTIONS (continued)

Module/ Calling Subroutine	Subroutine	Function
	CPCAL	Computes the hydraulic head or concentration distribution in aquitard soil columns.
	DXYGEN	Generates row and column coordinates of the rectangular mesh.
	EBFIND	Computes matrix bandwidths and determines the maximum bandwidth.
	EBFOR1	Computes seepage element matrices for rectangular elements.
	EBFOR2	Computes transport element matrices for rectangular elements.
	FILHED	Transfers head or concentration data for the final simulation time step to and from file unit number 8.
	FILVEL	Transfers velocity and saturated thickness data at each time step to and from file unit number 9.
	FILPLT	Transfers mesh data and simulation results to file unit number 10 for use in subsequent plotting.
	FILPRW	Performs output windowing and printing option.
	FIVEIO	Performs input/output operation of an integer array on a binary file with assigned unit number.
	FRVEIO	Performs input/output operation of a real array on a binary file with assigned unit number.
	HFINTP	Determines prescribed function and flux values for a particular time step using linear interpolation.
	MATMOD	Modifies the global matrix and right-hand-side vector to account for leakage fluxes between aquifers and confining aquitard.
	MESHGN	Generates nodal coordinates and element nodal connections for the specified rectangular grid.

Table 3-1. LIST OF SUBROUTINES BY MODULE AND A DESCRIPTION OF THEIR FUNCTIONS (continued)

Module/ Calling Subroutine	Subroutine	Function
	PBC	Allocates the prescribed Dirichlet and flux boundary conditions.
	QCAL	Computes nodal values of integrated fluid fluxes.
	RUPDAT	Updates values of recharge rate and integrated nodal values of recharge flux.
	SOLVEC	Solves a linear set of algebraic equations using Gauss elimination scheme for asymmetric banded matrix.
	SOLVEP	Solves a set of algebraic equations using a Gauss elimination scheme for symmetric banded matrix.
	SUPDAT	Updates values of solute (pesticide) application rate and integrated nodal values of solute mass flux.
	THUPDT	Updates saturated thickness of an unconfined aquifer.
	TRIMOD	Performs a direct solution of a tri-diagonal matrix equation using the Thomas algorithm.
	VARCAL	Performs a driving function by calling relevant subroutines to compute nodal values of head or concentration at the end of the current time step.
	VELCOM	Computes element centroidal values of Darcy velocity components (and nodal values of saturated thickness in the case of areal analysis).
MCARLO	BMPCHR	Capitalizes character variables.
	COMRD3	Reads and checks if input lines contain comments, data, or end of file.
	DECOMP	Decomposes correlation matrix into coefficient matrix required to generate correlated random numbers.

Table 3-1. LIST OF SUBROUTINES BY MODULE AND A DESCRIPTION OF THEIR FUNCTIONS (continued)

Module/ Calling Subroutine	Subroutine	Function
	EMPCAL	Generates empirically distributed random numbers by interpolating linearly from an input empirical distribution.
	ERRCHK	Writes error messages when unexpected end-of-file is encountered in input data file.
	EXPRN	Generates exponentially-distributed random numbers.
	FRQPLT	Writes plots of cumulative frequency distributions.
	FRQTAB	Writes tabulated cumulative frequency distributions.
	INITMC	Initializes statistical summation arrays, reorganizes Monte-Carlo input arrays to account for constant variables, and performs other miscellaneous Monte-Carlo initializations.
	LFTJUS	Left-justifies character variables (i.e., removes blanks from the left-side of character strings).
	LNGSTR	Finds the length of character variables (i.e., the number of non-blank characters).
	MCECHO	Writes Monte-Carlo input data to the shell output file.
	MTPV	Multiplies a vector of uncorrelated variables by a coefficient matrix to reform a vector of correlated variables.
	NAMFIX	Left-justifies and capitalizes character variables.
	NMB	Generates normally-distributed random numbers.
	OUTFOR	Writes frequency tables and plots.
	OUTPUT	Writes out statistical summaries of Monte-Carlo runs to the Monte-Carlo output file.
	RANDOM	Generates a vector of random numbers from specified distributions.

Table 3-1. LIST OF SUBROUTINES BY MODULE AND A DESCRIPTION OF THEIR FUNCTIONS (concluded)

Module/ Calling Subroutine	Subroutine	Function
	READM	Reads Monte-Carlo input data from a user-specified input file unit number.
	STATIS	Performs summations required to compute statistical moments for random model inputs and model outputs over all Monte-Carlo runs.
	STOUT	Computes statistical moments (mean, standard deviation, skewness, kurtosis, correlations, minimum and maximum) from summations computed by STATIS. Statistics are then written out to the Monte-Carlo output file.
	TRANSB	Transforms normally-distributed number to an SB distributed number.
	TRANSM	Transforms normally-distributed numbers to numbers having the appropriate user-specified distributions (i.e., log-normal SB, SU).
	UNIF	Generates uniform random numbers ranging between 0 and 1.

Table 3-2. COMMON BLOCK NAMES AND DESCRIPTIONS

Common Block	Description
ABOUN	Boundary condition variables.
ACCUM	PRZM cumulative terms carried from one time step to the next, primarily for outputting water and pesticide summaries.
ADISC	VADOFT coordinate and time-value arrays.
ASOLV	VADOFT solution arrays.
ATEMP	Temporary arrays for printing SAFTMOD boundary conditions.
BALANC	RUSTIC global mass balance terms.
BCDATA	SAFTMOD boundary condition data.
BDATA	SAFTMOD boundary condition data.
BNDOUT	SAFTMOD boundary sink term data.
BSOLV	VADOFT solution arrays.
CHAR	Character variables used in PRZM.
CHNEW	MONTE CARLO variable.
CNDF	PRZM accumulated number of days in each month (with and without leap year).
CONTR	VADOFT timekeeping and simulation control variables.
CONTR1	SAFTMOD simulation control parameters.
CONTR2	SAFTMOD simulation control variables.
CONTR3	SAFTMOD timekeeping and simulation control variables.
CONTR4	SAFTMOD simulation and output control data.
CONTR5	SAFTMOD control variables for boundary conditions.
CROP	PRZM crop timing and growth related terms.
ECHOIT	Information for RUSTIC output level.
ELSTOR	SAFTMOD solution matrix arrays.

Table 3-2. COMMON BLOCK NAMES AND DESCRIPTIONS (continued)

Common Block	Description
ESTORE	SAFTMOD aquifer geometry arrays.
FDATA	SAFTMOD flux data.GLOBPZGlobal mass balance data from PRZM.
GLOBRZ	Global mass balance variables.
GLOBSF	Global mass balance data from SAFTMOD.
GLOBVD	Global mass balance data from VADOFT.
HYDR	PRZM surface and soil hydrology related terms.
IN2SM	Transfer variables for input routines to computational routines of SAFTMOD.
IN2VAD	Decay rates, etc. of VADOFT chemicals.
INTDAT	SAFTMOD initial conditions arrays.
IRGT	PRZM irrigation related terms.
LNKSTO	Arrays used in linking VADOFT to SAFTMOD.
MASCON	Array to convert VADOFT dissolved to total concentrations.
MCVAR	PRZM variables related to MONTE CARLO.
MCRVAR	Parameters and random number arrays used in MONTE CARLO routines.
MCSTR	Storage of VADOFT/SAFTMOD outputs for MONTE CARLO.
MDATA	VADOFT material property data.
MDATAQ	SAFTMOD material property data.
MDATAT	SAFTMOD aquitard property data.
MET	PRZM meteorological related terms.
MISC	PRZM miscellaneous terms including output flags and time-keeping variables.
MSHDAT	SAFTMOD grid connectivity data.
MSHPAR	SAFTMOD grid coordinate data.

Table 3-2. COMMON BLOCK NAMES AND DESCRIPTIONS (continued)

Common Block	Description
NDSTOR	SAFTMOD aquifer geometry data (also contains an array to convert from dissolved to total concentration).
NDSTOS	SAFTMOD aquitard leakage data arrays.
PEST	PRZM pesticide fate, transport, and application related terms.
PRCNTR	SAFTMOD output control variables.
PRTCHK	Logical arrays to determine when VADOFT/SAFTMOD will write output.
PRZSTO	Storage of PRZM chemical fluxes and concentrations for linkage with VADOFT/SAFTMOD.
PTAP	PRZM/global mass balance solute input accumulator array.
RCHDAT	SAFTMOD recharge data.
RDATA	SAFTMOD chemical retardation and decay data.
RTDATA	SAFTMOD time varying recharge data.
SAZDAT	SAFTMOD time varying solute flux data.
SCHMDK	SAFTMOD chemical decay array.
SFTEXP	Decay ratio, etc. of SAFTMOD chemicals.
SFTSTO	SAFTMOD heads and concentrations.
SWHDA	VADOFT tabular data or permeability and pressure head versus water saturation.
TMDATA	SAFTMOD timekeeping data.
TRACE	RUSTIC program tracing variables.
TRACHR	Subroutine names used in RUSTIC trace.
TRIDIA	SAFTMOD coefficients for tridiagonal matrix solution.
VADSTO	VADOFT heads, fluxes, etc. for linkage w/SAFTMOD.
VASOLV	VADOFT tridiagonal matrix coefficient arrays.

Table 3-2. COMMON BLOCK NAMES AND DESCRIPTIONS (concluded)

Common Block	Description
VCHMDK	VADOFT chemical decay.
VDISC	SAFTMOD solution arrays for vertical aquitard columns.
VELEM	SAFTMOD velocity field data.
VONTR1	VADOFT simulation control data.
VONTR2	VADOFT mass balance variables.
VVELEM	Variables related to VADOFT nodal velocities.
VWORKM	VADOFT daughter products simulation arrays.
WAVE	SAFTMOD solution and matrix assembly arrays.
WAVE1	SAFTMOD matrix assembly arrays.
WAVE2	SAFTMOD matrix assembly arrays.
WELEM	VADOFT intermediate arrays for developing solution arrays.
WORKA	SAFTMOD matrix assembly variables.
WORKM	SAFTMOD temporary arrays for reading/writing scratch files.
WORKN	VADOFT residual saturation and capacity factor arrays.
WORKP	SAFTMOD daughter product simulation arrays.
WORKS	SAFTMOD temporary arrays for mass balance calculations.
ZONWHT	Weighting factors for linking PRZM/VADOFT/SAFTMOD pesticide zones.

Table 3-3. PARAMETER STATEMENTS UTILIZED IN THE RUSTIC CODE

Parameter	Description	Default Value	File Name
MCMAX	Maximum number of MONTE CARLO random input variables.	5	MCRVAR.CMN
MXMAT	Maximum number of VADOFT material types.	20	MXMAT.PRM
MXMBF	Maximum band width of SAFTMOD coefficient matrix.	62	MXMBF.PRM
MXMBW	Maximum band width of SAFTMOD coefficient matrix (transport) or maximum semiband width (flow).	62	MXMBW.PRM
MXNAQF	Maximum number of SAFTMOD aquifers.	2	MXNAQF.PRM
MXNBFV	Maximum number of SAFTMOD transient flux boundary conditions.	20	MXNBFV.PRM
MXNBHV	Maximum number of SAFTMOD transient Dirichlet boundary conditions.	20	MXNBHV.PRM
MXNBOU	Maximum number of SAFTMOD aquifer nodes where the net integrated flux values are required.	75	MXNBOU.PRM
MXNBTO	Maximum number of SAFTMOD steady-state Dirichlet boundary conditions.	100	MXNBTO.PRM
MXNCAT	Maximum number of SAFTMOD aquitard columns.	1250	MXNCAT.PRM
MXNCOL	Maximum number of SAFTMOD grid lines parallel to Y-axis.	75	MXNCOL.PRM
MXNCOW	Maximum number of SAFTMOD aquitard columns in an output window section.	30	MXNCOW.PRM
MXNDFL	Maximum number of SAFTMOD steady-state flux model boundary conditions.	50	MXNDFL.PRM
MXNE	Maximum number of SAFTMOD elements in the aquifer mesh.	400	MXNE.PRM
MXNLAY	Maximum number of VADOFT layers. A VADOFT layer is a collection of contiguous elements having a uniform material type.	20	MXNLAY.PRM
MXNMAD	Maximum number of aquitard materials.	10	MXNMAD.PRM

Table 3-3. PARAMETER STATEMENTS UTILIZED IN THE RUSTIC CODE (continued)

Parameter	Description	Default Value	File Name
MXNMAT	Maximum number of SAFTMOD aquifer materials.	20	MXNMAT.PRM
MXNNDW	Maximum number of SAFTMOD nodes in an output window section.	30	MXNNDW.PRM
MXNOBS	Maximum number of SAFTMOD observation nodes where monitoring of head or concentration values is desired.	24	MXNOBS.PRM
MXNOD	Maximum number of VADOFT nodes.	120	MXNOD.PRM
MXNP	Maximum number of SAFTMOD nodes.	470	MXNP.PRM
MXNPAT	Maximum total number of SAFTMOD nodes in an aquitard.	4000	MXNPAT.PRM
MXNPCO	Maximum number of SAFTMOD nodes per finite element column in an aquitard.	20	MXNPCO.PRM
MXNPSZ	Maximum number of nodes per SAFTMOD solute flux zone.	150	MXNPSZ.PRM
MXNRC	The maximum of MXNCOL and MXNROW.	75	MXNRC.PRM
MXNROW	Maximum number of SAFTMOD grid lines parallel to X-axis.	75	MXNROW.PRM
MXNRZ	Maximum number of nodes per recharge zone (used in global mass balance).	450	MXNRZ.PRM
MXNRZO	Maximum number of SAFTMOD recharge zones.	4	MXNRZO.PRM
MXNSZO	Maximum number of SAFTMOD solute application zones.	4	MXNSZO.PRM
MXNTCL	Maximum number of SAFTMOD time values at which head or concentration values at selected nodes are to be printed.	40	MXNCL.PRM
MXNTNF	Maximum number of SAFTMOD values on the graph of time vs. flux at a transient flux node (not used in linked simulation).	25	MXNTNF.PRM
MXNTNH	Maximum number of SAFTMOD values on the graph of time vs. head or concentration at a transient Dirichlet node (not used in linked simulation).	25	MXNTNH.PRM

Table 3-3. PARAMETER STATEMENTS UTILIZED IN THE RUSTIC CODE (continued)

Parameter	Description	Default Value	File Name
MXNTRP	Maximum number of SAFTMOD interpolation control points on the graph of recharge rate (not used in linked simulation).	60	MXNTRP.PRM
MXNTS	Maximum number of SAFTMOD time steps (not used in linked simulation).	200	MXNTS.PRM
MXNTSZ	Maximum number of SAFTMOD interpolation control points on the graph of solute mass application rate versus time (not used in linked simulation).	100	MXNTSZ.PRM
MXPRT	Maximum number of VADOFT observation nodes.	1	MXPRT.PRM
MXTIM	Maximum number of VADOFT iterations necessary for problem solutions.	30	MXTIM.PRM
MXTMV	Maximum number of VADOFT time interpolation values.	30	MXTMV.PRM
MXVDT	Maximum number of VADOFT timesteps (days) per SAFTMOD simulation.	31	MXVDT.PRM
MXWNDO	Maximum number of SAFTMOD output window sections.	10	MXWNDO.PRM
NAPP	Maximum number of PRZM pesticide applications.	10	PARM.INC
NC	Maximum number of PRZM cropping periods.	5	PARM.INC
NCMPTS	Maximum number of PRZM compartments in the soil profile.	118	PARM.INC
NCMAX	Maximum number of MONTE CARLO variables for which cumulative distributions are plotted.	3	MCRVAR.CMN
NEMP	Maximum number of MONTE CARLO empirical distribution points.	20	MCRVAR.CMN
NMAX	Maximum number of MONTE CARLO summary output variables.	8	MCRVAR.CMN
NMXFIL	Maximum number of files which can be open at one time.	20	IOUNITS.PAR
NPMAX	Maximum length of MONTE CARLO output averaging periods.	5	MCRVAR.CMN

Table 3-3. PARAMETER STATEMENTS UTILIZED IN THE RUSTIC CODE (concluded)

Parameter	Description	Default Value	File Name
NRMAX	Maximum number of MONTE CARLO runs.	2000	MCRVAR.CMN
NPII	Maximum number of PRZM particles used in MOC algorithm.	600	PARM.INC

3.8 DATA BASES

There are currently under development, four data bases which will be available for use with the RUSTIC code in the future: a meteorological data base, a geographic soils data base, a soils properties and cropping practices data base, and a descriptive statistics data base for Monte Carlo simulation (Carsel 1988, personal communication). These data bases will be useful in assisting the user to select appropriate model parameters and input time series data. The data bases should be available in late 1989 from the Environmental Protection Agency, Environmental Research Laboratory in Athens, Georgia (Carsel 1989, personal communication).

SECTION 4

MODEL BUILDING

In this section, the steps which are preliminary to actual model application are discussed. It is not meant to be a general treatise on modeling, but instead it will offer some specific guidance applicable to RUSTIC. The experienced model user may want to skip the first part of this section which deals with such concepts as problem definition, idealizing the physical system, etc., and proceed directly to the description of the input data sequence and format. However, for some, the review of these concepts may prove valuable.

4.1 SYSTEM ABSTRACTION

In order to model a natural system, which is inherently complex, the model user must idealize or abstract certain aspects of it. As a basic first step, it is essential to find out as much as one can about the system and to formulate a mental "model" of how it functions. Simultaneously, the user must have in mind a set of goals for the modeling exercise and must keep in mind the limitations of the model. The intersection of modeling goals, model capabilities and the "reality" of the natural system (including the data available to describe it) form the background for the model application. Hopefully, Sections 1 and 3 have given the user an understanding of the capabilities of the RUSTIC model. It remains to idealize the system, translate that abstraction into a model configuration, formulate a simulation strategy, estimate parameters, and execute the model.

4.1.1 Idealizing the System

The RUSTIC code is capable of representing very simple or fairly complex subsurface systems. As previously discussed, it has three modules: PRZM, which simulates pesticide fate and transport in the crop root zone; VADOFT, which simulates pesticide fate and transport between the crop root zone and the water table; and SAFTMOD, which simulates fate and transport in the saturated zone. If the water table is close to the crop root zone and the root zone soils are fairly permeable, then the user may choose to exclude VADOFT from the simulation. If it can be done, this offers two advantages:

- it eliminates the possibility of nonconvergence of VADOFT flow algorithms and

- it will speed up model execution time.

If the system has a thick vadose zone with relatively slow draining soils, then the use of VADOFT is essential to overcome the limitations of the elementary soil hydraulics in PRZM.

PRZM and VADOFT are one-dimensional models and formulated so that vertical material layering can be accounted for. In PRZM, these material zones are referred to as horizons, while in VADOFT, they are referred to as material layers. The maximum number of materials is controlled by a parameter statement in each model.

The user may want to differentiate horizons or material layers for several reasons. There may be differences, for instance, in hydraulic properties which would affect water transmission rates, organic carbon content which would affect solute adsorption, or soil pH which might affect chemical degradation by hydrolysis. In PRZM, both water and chemical properties are entered for each horizon. In VADOFT, however, the user has the option of specifying a different material layering for flow simulations and for transport simulations. For example, in VADOFT, the user may specify one material layer for flow and three material layers for transport. In PRZM, for the same case, the user would have to select three horizons to differentiate the transport properties, and enter the same set of hydraulic properties redundantly for these horizons.

Spatial heteorgeneities can be addressed by using Monte Carlo simulation. Although the multiple application of PRZM and/or VADOFT modules is currently not implemented, water and solute fluxes to SAFTMOD may be specified over different areas or lengths.

With SAFTMOD, the user can allow for both lateral and vertical heterogeneity. The user may simulate a one- or two-aquifer system with an intervening aquitard. Laterally, the user can specify "material zones" which may have porous media with contrasting properties. The user also has the capability to specify recharge zones, or pesticide flux zones at SAFTMOD upper boundary nodes. This capability allows the user to translate the nonuniformity in water and solute flux to the saturated zone represented by SAFTMOD.

SAFTMOD is a two-dimensional model and is capable of being run in an X-Y, X-Z or axisymmetric configuration. The user must decide which configuration best meets the modeling goals and concurrently, best describes the real system. Decision trees for aiding the user in selecting a configuration are shown in Figures 4.1 and 4.2. Figure 4.1 shows options for simulating flow, while 4.2 shows options for solute transport configurations. The terms "radius of influence" (small, medium, or large) and "full or partial penetration," of course, refer to the interaction of the well with the aquifer system. In order for the flow and solute transport models to interact properly, they must both be configured the same way (e.g., both 2-D, X-Z). The decision trees were designed for use with rather simple systems and may not be appropriate when idealizing complex groundwater systems.

As an example, in Figure 4.1, suppose that the system is an unconfined surficial aquifer in which the well has a large radius of influence. This suggests that the regional flow pattern is dominated by the gradients induced

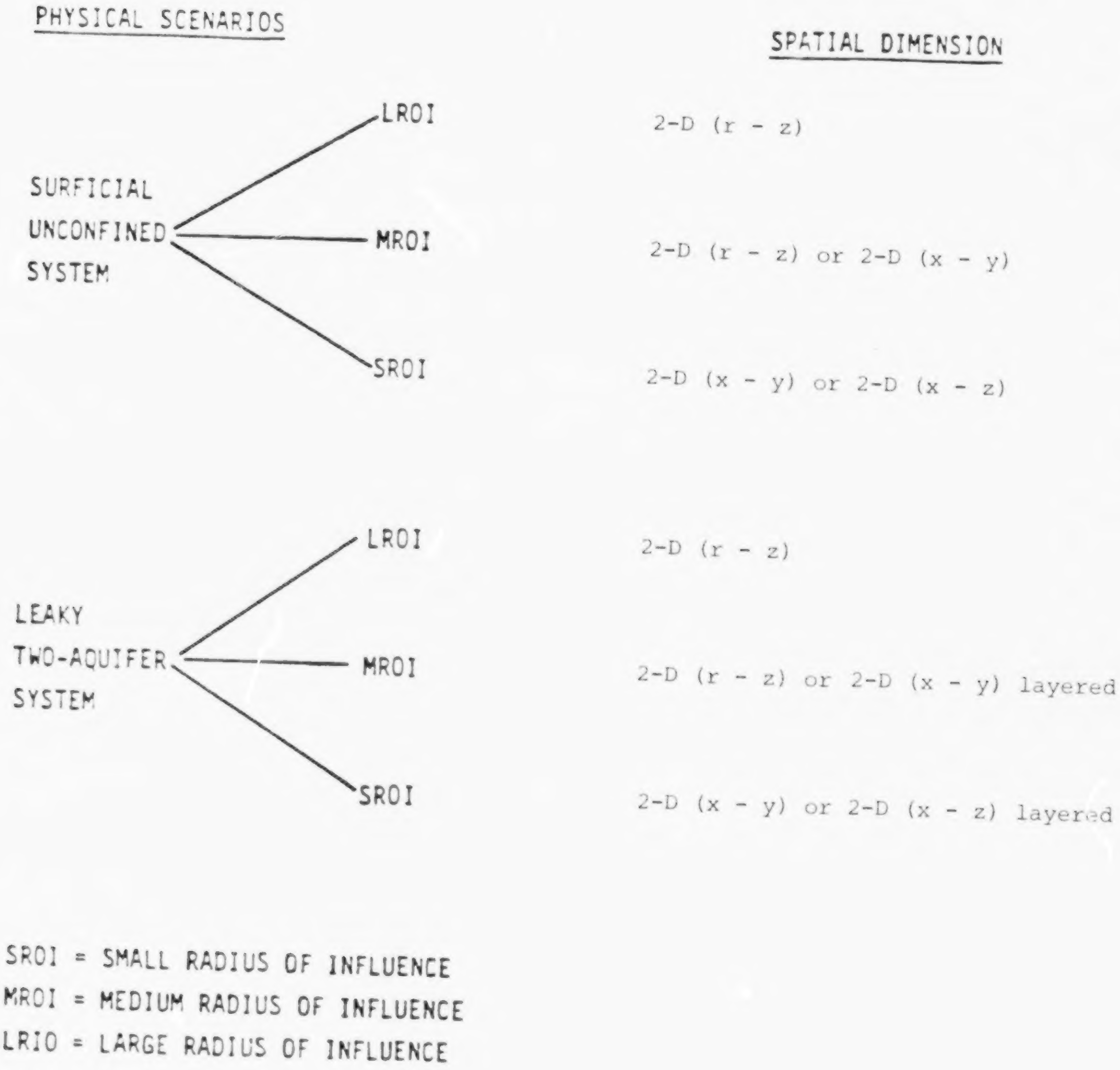
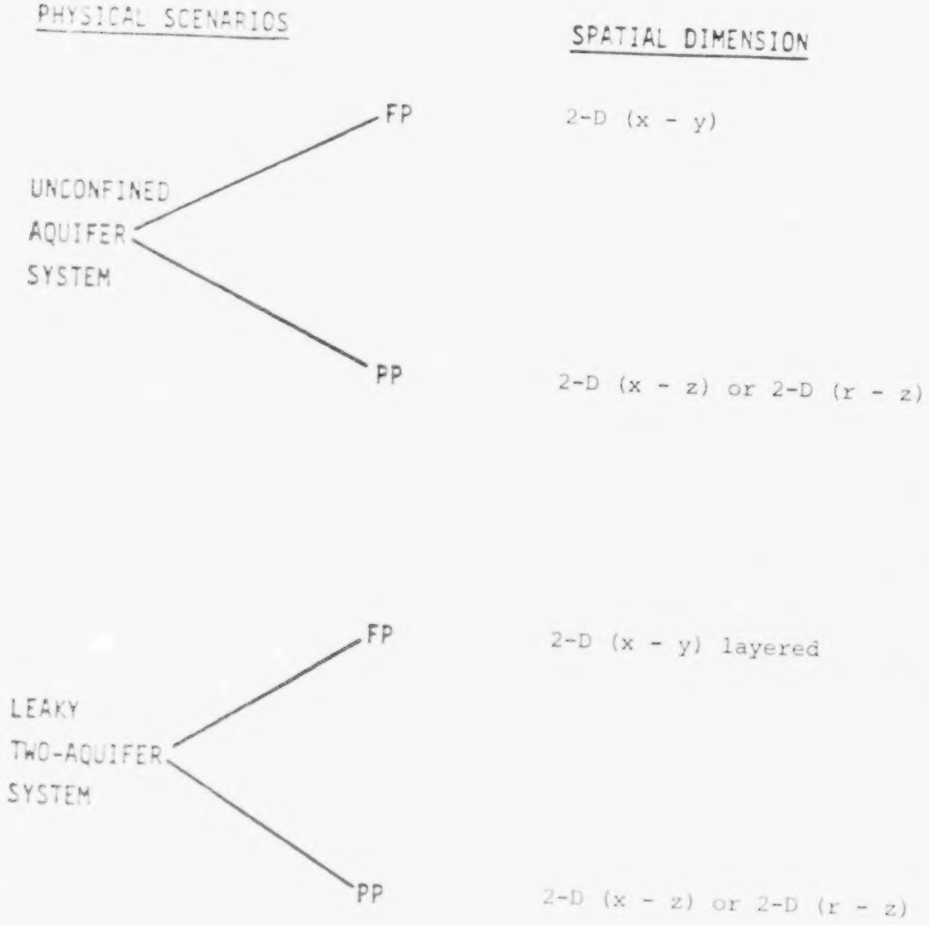

PHYSICAL SCENARIOS
SPATIAL DIMENSION
SURFICIAL UNCONFINED SYSTEM
LROI
2-D (r - z)
MROI
2-D (r - z) or 2-D (x - y)
SROI
2-D (x - y) or 2-D (x - z)
LEAKY TWO-AQUIFER SYSTEM
LROI
2-D (r - z)
MROI
2-D (r - z) or 2-D (x - y) layered
SROI
2-D (x - y) or 2-D (x - z) layered
SROI = SMALL RADIUS OF INFLUENCE
MROI = MEDIUM RADIUS OF INFLUENCE
LRIO = LARGE RADIUS OF INFLUENCE

Figure 4.1. Decision tree for groundwater flow scenarios.


PHYSICAL SCENARIOS
SPATIAL DIMENSION
UNCONFINED AQUIFER SYSTEM
FP
2-D (x - y)
PP
2-D (x - z) or 2-D (r - z)
LEAKY TWO-AQUIFER SYSTEM
FP
2-D (x - y) layered
PP
2-D (x - z) or 2-D (r - z)

FP = FULLY PENETRATING
PP = PARTIALLY PENETRATING

Figure 4.2. Decision tree for solute transport scenarios.

by well pumping and, therefore, an axisymmetric analysis is appropriate. If, on the other hand, the well has a small radius of influence, then the regional gradient is dominant and an X-Y (plan view) simulation is suggested. Similarly, if the well only partially penetrates the aquifer (inducing selective withdrawal from the upper part of the aquifer and vertical velocities) then an R-Z (axisymmetric) simulation could be used for transport (see Figure 4.2). However, if the R-Z axisymmetric grid is used for transport, it must also be used for flow.

In addition to decisions involving the configuration of the grid, the user must decide whether to consider recharge of water to SAFTMOD in the analysis. Obviously, there are situations in which this may be important to the analysis and situations in which it will not be. For instance, in a thick aquifer in which the recharge produces only minor fluctuations in the water table elevations, the error caused by not considering recharge will be small. This is especially true where the pumping will fully penetrate the aquifer or where an X-Y simulation is used (concentrations will be averaged over the entire aquifer thickness). On the other hand, for shallow aquifers in which the well is screened in the top of the formation, water table fluctuations could have a sizeable impact on the resulting concentrations in the pumping well.

4.1.2 Grid Specification

Once the configuration of the model is decided upon, the next step is to set up the grid systems for each of the models. In PRZM, the user may select various sizes of soil layers (think of the midpoints of these layer thicknesses as nodes) by horizon. If a volatile chemical is being simulated, it is suggested that a fine nodal spacing be chosen near the soil surface as the simulation of the pesticide concentration gradient here is very important (see Volume I, Section 2). In this case, the top 20 cm or so should have layers (i.e., nodal spacing) from 0.5 to 1 cm in thickness. For nonvolatile chemicals, this near surface definition is less important. Nodal spacing in PRZM or in VADOFT can be wider where solute velocities are higher. However, nodal spacings which are too wide can lead to oscillations in the solution surface.

In designing a finite element grid for variably saturated flow simulations, one should select nodal spacings that will yield reasonable approximations to the expected moisture profiles. Small nodal spacings should be used in the zones where head gradients or moisture fronts are steep. The nodal spacings may be gradually increased in the zone where no abrupt changes in hydraulic conductivities occur and the head gradients are gradually sloping. The variably saturated flow simulation can be performed using either the Picard or the Newton-Raphson solution algorithm, or a Newton-Raphson algorithm modified by Huyakorn (1987, personal commnication). For one-dimensional cases where convergence difficulties are not expected, the efficiency of these three algorithms has been found to be similar. For certain steady-state cases involving higher nonlinear soil moisture characteristics, the use of either Newton-Raphson algorithm is preferable, particularly when the Picard algorithm fails to converge within a reasonable number of iterations (say between 10 and 20). Experience with the VADOFT code indicates that when running in the linked mode, the modified Newton-Raphson method, (i.e., INEWT = 2) should be used for the iteration procedure.

In designing a finite element grid for transport simulations, one should select nodal spacings that will yield reasonable approximations to the expected concentration distributions. The selection of nodal spacing (Δz) and time step value (Δt) should follow the so-called Peclet number and Courant number criteria where possible. These two criteria are given as follows:

$$\frac{\Delta z}{\alpha_L} \leq 4 \text{ (Peclet number)} \tag{4-1}$$

$$V_{sol}\ \Delta t/\Delta z \leq 1 \text{ (Courant number)} \tag{4-2}$$

where

$$V_{sol} = V/\theta R \tag{4-3}$$

where α_L is the longitudinal dispersivity, V_{sol} is the solute velocity, V is the Darcy velocity, θ is the water content, and R is the retardation coefficient.

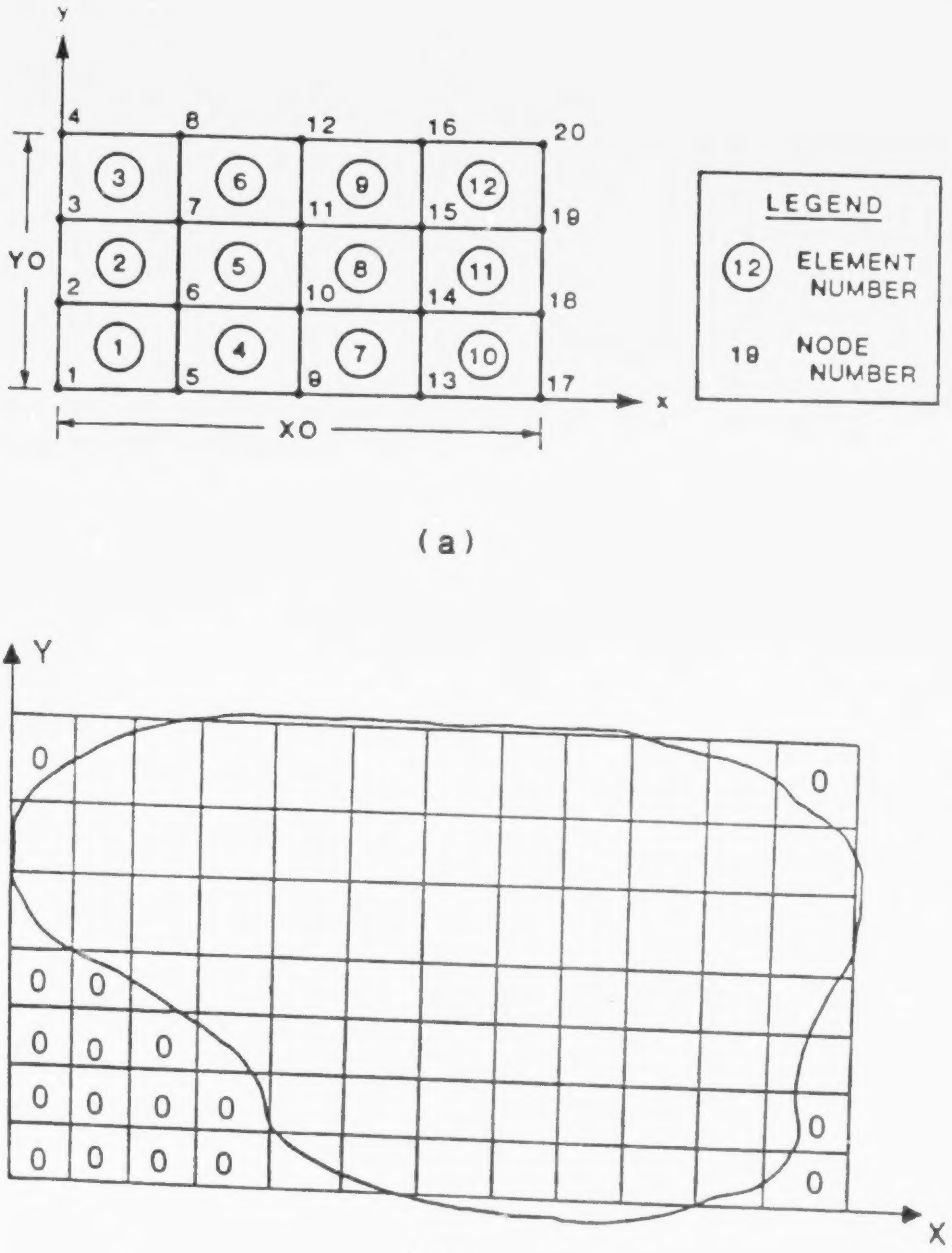
The VADOFT code also provides the user with the option of using upstream weighting to curb numerical oscillations that may occur in solving the advective-dispersive transport equation. The recommended value of ω, the weighting factor, is determined by using the following formulae:

$$\omega = 1 - 4\alpha_L/\ell, \qquad \ell > 4\alpha_L \tag{4-4}$$

$$\omega = 0 \qquad , \qquad \ell \leq 4\alpha_L \tag{4-5}$$

where α_L is the longitudinal dispersivity, and ℓ is the length of the element.

Spatial discretization of the solution region is performed automatically in the SAFTMOD code given user instructions. A rectangular grid (Figure 4.3) is used to represent the modeled two-dimensional region. In a cross-sectional or an axisymmetric analysis, the modeled region corresponds to the entire system, which is considered as one unit where different materials are accommodated by assigning different sets of material properties for different elements. In an areal analysis, a distinction is made between aquifer and aquitard regions. Each aquifer region is discretized using a network of rectangular elements. The same nodal arrangement and element configurations are used for different aquifers. Nodes and elements are numbered


y
x
YO
XO
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
LEGEND
12 ELEMENT NUMBER
19 NODE NUMBER
Y
X
0

(a)

(b)

Figure 4.3. Discretization of aquifer regions: (a) regular region, and (b) irregular region.

sequentially as shown in Figure 4.3a. An irregular boundary is accommodated by assigning zero material number to elements outside the region of interest (Figure 4.3b). In the areal simulation of a system comprising two aquifers separated by an aquitard, numbering of nodes and elements is performed, aquifer by aquifer, starting from the bottom aquifer. The confining aquitard region is treated as a series of vertical columns each of which is bounded at both ends by two opposite aquifer nodes. Each aquitard column is represented by a one-dimensional linear finite element grid. The one-dimensional grid is generated automatically using a local dimensionless vertical coordinate, ξ,defined as $\xi = z'/b'$, where z' is the height measured from the bottom of the aquitard, and b' is the thickness of the aquitard column. Aquitard nodes in the column are numbered sequentially from the bottom to top of the column.

One of the requirements of the linkage of either PRZM or VADOFT to SAFTMOD is the overlap of model spatial domains to provide for continuity and realistic simulation at model interfaces. This is discussed in some detail in Section 5 of Volume I. When SAFTMOD is used in a 2D X-Y configuration, the PRZM or VADOFT grid should extend through the saturated zone to the base of the uppermost aquifer. It is suggested that the nodal spacing be relatively close in the zone in which the water table is fluctuating. This will allow for more accurate interpolation of solute flux to the saturated zone. Below this zone, the user can space the nodes more widely, as the results of the vertical simulation below the water table in the X-Y SAFTMOD configuration are meaningless and close spacing in this region will increase execution time. The user should use nodal spacing, however, sufficiently close to curb numerical oscillations. In the X-Z or axisymmetric simulation of the saturated zone, the PRZM or VADOFT grid should also extend to the base of the uppermost aquifer.

Once the model configuration and grid layout is decided upon, the user can begin to build parameter files, which is the subject of the next section.

4.2 DESCRIPTION OF INPUT SEQUENCES

In the following sections, the input sequences for the Execution Supervisor, PRZM, VADOFT, SAFTMOD and MCARLO are discussed. All of the input files to these modules, except for the meteorological data file, may have embedded comment lines. A comment line is any line beginning with three adjacent asterisks ('***'). These comment lines are ignored by the code.

4.2.1 Execution Supervisor

This section describes the development of the input data file of the execution supervisor. This file is used to define: 1) which options are to be selected for a simulation, 2) the file names to be used for input and output, and 3) certain globally-defined data (e.g., the start and end dates of the simulation). This file, RUSTIC.RUN, is the only input data file which may not have an optional (user-selected) name or path (i.e., the file must be located in the default directory). An example execution supervisor input file is shown in Figure 4.4. Its components are discussed below.

```
PRZM                    ON
VADOFT                  OFF
SAFTMOD                 ON
MONTE CARLO             ON
TRANSPORT SIMULATION    ON
ENDRUN
  *** INPUT FILES
  PATH                  D:\SU\EPAB3\DATA\ONECHM\
  METEOROLOGY           MD1.DAT
  PATH                  C:\EPAB3\EXESUP\RUSTIC\DATA\CHKRATES\
  SAFTMOD INPUT         SINXZWR.DAT
  PATH                  C:\EPAB3\EXESUP\RUSTIC\DATA\CHKELEV\
  VADOFT INPUT          VIN.DAT
  PRZM INPUT            P2VLNK.DAT
  MCIN                  @RANDU.IN
  *** output files
  PATH                  D:\RUSTIC\TEST\
  TIME SERIES           KFLTS.PRN
  MCOUT                 MCOUT.PRN
  MCOUT2                MCOUT2.PRN
  PRZM OUTPUT           POUT.PRN
  SAFTMOD OUTPUT        SOUT.PRN
  VADOFT OUTPUT         VOUT.PRN
  *** SCRATCH FILES
  VADOFT TAPE10         DUMT10
  PRZM RESTART          RESTART.DUM
  SAFTMOD TAPE8         TAPE8
  SAFTMOD TAPE9         TAPE9
  SAFTMOD TAPE10        TAPE10
ENDFILES
  START DATE            020177
  END DATE              020178
  TIME STEP             15
  NUMBER OF CHEMICALS   1
  PARENT OF 2           1
  PARENT OF 3           2
ENDDATA
ECHO                    ON
TRACE                   OFF
```

Figure 4.4. Example Execution Supervisor Input File (RUSTIC.RUN)

4.2.1.1 Option Records--

All of the potential options have default values and, if an option is not specifically set, the default value will be assumed. These defaults are as follows: PRZM=ON, VADOFT=OFF, SAFTMOD=OFF, MONTE CARLO=OFF, and TRNSIM (simulate solute transport)=OFF. The options section must end with ANAME="ENDRUN" (see Table 4-1) even if all of the default values are to be used.

4.2.1.2 File Records--

The file records (EXESUP2) of the execution supervisor input are used to assign the user supplied names and locations of the files required for a simulation to the appropriate RUSTIC file. If files are defined within these records which are not necessary because of the options selected in the options records (EXESUP1), the file name is ignored.

4.2.1.3 Global Parameters Records--

The global parameters records (EXESUP3) are used to define certain environmental and simulation control parameters which need to be defined for all phases of the simulation. These parameters include the start and end dates, the number of days per SAFTMOD timestep (NLDLT), the number of chemical species being simulated (NCHEM), and the index number of the parent species for each chemical species being simulated (IPARNT(ICHEM)).

NLDLT is required only if SAFTMOD is on. If NLDLT is set larger than the total number of days of the simulation, the code issues a warning and resets NLDLT to the total number of days.

The number of chemicals being simulated (NCHEM) must be defined if TRNSIM is ON. Values of 1, 2, or 3 are valid. If NCHEM is greater than 1, the parent species index number must be provided. Chemical 1 can have no parent; the code assumes this and the user does not have to specify it. Chemical 2 can have no parent (IPARNT[2]=0) or can have chemical 1 as a parent (IPARNT[2]=1). Chemical 3 can have no parent or can have chemical 1 or 2 as the parent species.

4.2.1.4 Trace Level Record--

The trace level record (EXESUP4) is, in general, only necessary for debugging problems with a simulation. If the trace level is set to a value greater than one, the subroutine that RUSTIC is currently executing during a simulation, as well as the path of subroutine calls to access that subroutine, are displayed on the standard output device. A trace can be useful for debugging a simulation but, when used, can increase execution time considerably. If the trace level record is not included in the EXESUP data set, a default value of 3 is assumed. A value of 3 indicates that subroutine calls three levels deep will be displayed. For example, if RUSTIC calls subroutine "A" which calls subroutine "B" which calls subroutine "C" which calls subroutine "D," the string "RUSTIC>A>B>C" will be displayed while "C" is being executed and while "D" is being executed since the call to "D" is greater than 3 levels deep.

Table 4-1. INPUT FORMATS FOR THE EXECUTION SUPERVISOR MODULE (EXESUP)

Variable	Description		Units
OPTION RECORDS EXESUP1 -- ANAME, STATS FORMAT(A24,A56)			
ANAME	Name of simulation option which can be one of the following list:		--
	Value	Module or variable	
	'PRZM'	Pesticide/Root Zone	
	'VADOFT'	Vadose Zone	
	'SAFTMOD'	Saturated Zone	
	'TRNSIM'	Solute Transport	
	'MONTE CARLO'	Monte Carlo module	
	'ENDRUN'	End of option's selection	
STATS	Either "ON" or "OFF" for the modules. The following are the default values which are assumed if the module status is not explicitly defined.		
	Module	Stats	
	PRZM	ON	
	VADOFT	OFF	
	SAFTMOD	OFF	
	TRNSIM	OFF	
	MONTE CARLO	OFF	
FILE RECORDS EXESUP2 -- ANAME, FNAME FORMAT(A24,A56)			
ANAME	Label defining which input or output file is being defined. The following values of ANAME can be used and must be present if they are required.		--

Table 4-1. INPUT FORMATS FOR THE EXECUTION SUPERVISOR MODULE (EXESUP) (continued)

Variable	Description	Units
Value	When Required	File Represented
'PATH'	never required but is available as a convenience in defining file location	Path for following files.
'METEOROLOGY'	always	Meteorological data (time series) input file.
'PRZM INPUT'	PRZM is ON	PRZM definition input file.
'SAFTMOD INPUT'	SAFTMOD is ON	SAFTMOD definition input file.
'VADOFT INPUT'	VADOFT is ON	VADOFT definition input file.
'MCIN'	MONTE CARLO is ON	Monte Carlo simulation definition (input) file.
'PRZM OUTPUT'	PRZM is ON and MONTE CARLO is OFF	PRZM hydrology, pesticides, and concentrations output file.
'TIME SERIES'	PRZM is ON and MONTE CARLO is OFF	PRZM time series output file.
'SAFTMOD OUTPUT'	SAFTMOD is ON	SAFTMOD output file.
'VADOFT OUTPUT'	VADOFT is ON	VADOFT output file.
'MCOUT'	MONTE CARLO is ON	Monte Carlo output summary.
'MCOUT2'	MONTE CARLO is ON	Monte Carlo output of individual simulations.
'SAFTMOD TAPE8'	SAFTMOD is ON	Unformatted file with the nodal values of concentrations completed at final time step.

Table 4-1. INPUT FORMATS FOR THE EXECUTION SUPERVISOR MODULE (EXESUP) (continued)

Variable	Description	Units
Value	When Required	File Represented
'SAFTMOD TAPE9'	SAFTMOD is ON	Unformatted file with velocity and saturated thickness data.
'SAFTMOD TAPE10'	SAFTMOD is ON	Unformatted file with Darcy velocities and nodal fluxes.
'VADOFT TAPE10'	VADOFT is ON and TRNSIM is ON	Unformatted file with nodal values of element Darcy velocity components and water-phase saturation.
'PRZM RESTART'	PRZM is ON	Unformatted file with intermediate PRZM data values. Used to restart PRZM from previous simulation.
'ENDFILES'	Always - at end of file definition - to indicate that all necessary files have been defined.	--
FNAME	The name of the file defined by ANAME. If the path of a previous PATH record is to be ignored, the first character of FNAME must be '@'. If FNAME is a path (i.e., ANAME was defined as 'PATH'), it should end with the character '\' (for MSDOS microcomputers).	--

Table 4-1. INPUT FORMATS FOR THE EXECUTION SUPERVISOR MODULE (EXESUP) (continued)

Variable	Description	Units
GLOBAL PARAMETERS RECORDS EXESUP3--ANAME, FNAME FORMAT(A24,A56)		
ANAME	Label defining which global parameter is being defined. The following values of ANAME can be used and must be present if they are required.	--

Value	When Required	Comments
'START DATE'	Always	Indicates that the date of the start of simulation will be present in the FNAME field.
'END DATE'	Always	Indicates that the date of the end of simulation will be present in the FNAME field.
'TIME STEP' (NLDLT) will be in	If SAFTMOD is on the FNAME	Indicates that the time step field.
'NUMBER OF CHEMICALS'	If TRNSIM is on	Indicates that the number of chemicals will be in the FNAME field.
'PARENT OF n'	If TRNSIM is on and NUMBER OF CHEMICALS greater than 1	Indicates that the index of the parent species of this chemical (n should be 1, 2, or 3) will be in the FNAME field.
'ENDDATA'	Always - at the end of global parameters definition	

Table 4-1. INPUT FORMATS FOR THE EXECUTION SUPERVISOR MODULE (EXESUP) (continued)

Variable	Description	Units
FNAME	Integer values with the following formats dependent on the value of ANAME	--

ANAME	Variable	Description	Format
'START DATE'	ISDAY, ISMON, ISTYR	Starting day, month, year	(3I2)
'END DATE'	IEDAY, IEMON, IEYR	Ending day, month, year	(3I2)
'TIME STEP'	NLDLT	Number of days per SAFTMOD simulation	(BN,I56)
'NUMBER OF CHEMICALS'	NCHEM	Number of chemicals to be simulated in a transport simulation	(BN,I56)
'PARENT of n'	IPARNT(n)	Index of the parent species chemical n [n is read with the format (BN,I25)]	(BN,I56)

ECHO LEVEL RECORD EXESUP4 (optional)--ANAME, STATS
FORMAT(A24,A56)

ANAME	The label 'ECHO'	--
STATS	Either 'ON' or 'OFF' or an integer between 0 and 9. If an integer, it is read with FORMAT (BN,I56)	--

Table 4-1. INPUT FORMATS FOR THE EXECUTION SUPERVISOR MODULE (EXESUP) (concluded)

Variable	Description	Units
TRACE LEVEL RECORD EXESUP5 (optional)--ANAME, STATS FORMAT(A24,A56)		
ANAME	The label 'TRACE'	--
STATS	Either 'ON' or 'OFF' or an integer value. If an integer, it is read with FORMAT (BN,I56)	--

4.2.1.5 Echo Level Record--
The echo level record (EXESUP5) allows the user to determine how much data will be written to the output echo file and to the VADOFT and SAFTMOD output files. This record is available as a convenience to the user and allows the user to obtain more information when debugging a simulation. It also allows the user to speed up a simulation and reduce the size of output files during a production simulation. If this record is not supplied in the EXESUP data set, a default value of 5 will be assumed if MONTE CARLO is off (1 if MONTE CARLO is on).

Table 4-2 demonstrates the effect of the echo level on the output of the execution supervisor. An 'x' in the table signifies that the output feature is enabled with the listed value of echo level. As an example in using this table, a subroutine trace will be written to the standard output device if an echo level of 4 or greater is selected (note that if the trace level is set to 0, the subroutine trace will not appear even if the echo level is greater than or equal to 4).

An echo level of 8 or 9 is useful during the early stages of defining a simulation. An echo level of 8 (or 9) will result in a trace of which line the code is attempting to read (for example, the line "Reading record [7a]" would appear in the output echo file as the code attempts to read SAFTMOD group 7a). SAFTMOD group 7a is required as a function of options defined earlier in the SAFTMOD input stream, and it might be possible that the user thought that the options were set such that group 7a was not required. Thus, an echo level of 8 or 9 is useful for defining what the code is actually trying to read versus what the user expects the code to be reading.

An echo level of 9 will result in a trace of each line being read in by the code to appear in the output echo file before that line is interpreted as data. This is useful for displaying typographical errors which the user may have made in developing an input file. For example, if the user had

Table 4-2. THE EFFECT OF THE ECHO LEVEL ON THE OUTPUT OF EXESUP

Output Feature	Echo Level									
	0	1	2	3	4	5	6	7	8	9
Percent complete bar graph*		X	X	X	X	X	X	X	X	X
Simulation status write to screen			X	X	X	X	X	X	X	X
Simulation status write to output echo file				X	X	X	X	X	X	X
Subroutine trace available					X	X	X	X	X	X
Warnings written to screen and output echo file						X	X	X	X	X
Results of linkage routines written to output echo file							X	X	X	X
Additional data on simulated values of water/solute flux written to output echo file								X	X	X
Additional data on simulated values of head/concentrations written to output echo file									X	X
Echo of which line is currently being read									X	X
Echo of image of the line which is currently being read										X

* Applies to IBM PC compatible computers.

inadvertently inserted a character within a data field which was to be read as a real number, the echo of the line displaying the faulty data field would appear before the fatal error message which would result when that field was being interpreted as a real number.

Lower values of the echo level are useful for speeding up a simulation and for reducing the amount of output. The amount of output generated by EXESUP, VADOFT, and SAFTMOD is controlled by the echo level. The amount of PRZM output is controlled by defining the output frequency of hydrology, concentration, and pesticide results (see Section 4.2.2).

The effect of the echo level on the data output of EXESUP, VADOFT, and SAFTMOD is defined in Table 4-3. At a level of 4 or greater, the results of mass balance calculations become available (global mass balance as calculated by EXESUP and the internal mass balance calculations of VADOFT and SAFTMOD). At a level of 5 or greater, the results of the calculations at VADOFT and/or SAFTMOD observation nodes are printed. Note that observation nodes must be defined for VADOFT and/or SAFTMOD using the input file options described for these modules (see Sections 4.2.3 and 4.2.4).

Table 4-3. THE EFFECT OF THE ECHO LEVEL ON THE OUTPUT OF EXESUP, VADOFT, AND SAFTMOD

Data Group	Echo Level									
	0	1	2	3	4	5	6	7	8	9
Mass balance results					X	X	X	X	X	X
Results at observation nodes						X	X	X	X	X
Standard output							X	X	X	X

Echo levels less than 4 are generally only of use when using the Monte Carlo simulation option since most of EXESUP, and all of PRZM, VADOFT, and SAFTMOD output will be suppressed.

Table 4-4 presents the relative time of execution as a function of the echo and trace levels. These times are relative to the execution time of a 2-month deterministic run (MONTE CARLO = 'OFF') using the defaults ECHO = ON and TRACE = OFF.

Table 4-4. RELATIVE EXECUTION TIMES AS A FUNCTION OF ECHO LEVEL AND TRACE LEVEL (PRZM = ON, VADOFT = ON, SAFTMOD = ON, MONTE CARLO = OFF, TRNSIM = ON)

Trace Level	Echo Level				
	0 (OFF)	4	5 (ON)	6	9
0 (OFF)	0.97	1.00	1.00	1.09	1.21
3 (ON)	--	1.64	1.65	1.72	1.82
5	--	2.30	2.35	2.43	2.50

Table 4-5 presents the relative file sizes which result from selected values of the echo level. The file sizes are relative to the file sizes which resulted from the simulation described above.

Table 4-5. RELATIVE OUTPUT FILE SIZES AS A FUNCTION OF ECHO LEVEL

	Echo Level				
	0 (OFF)	4	5 (ON)	6	9
Output Echo	0.83	0.95	1.00	1.29	1.80
PRZM Output	0	1.00	1.00	1.00	1.00
VADOFT Output	0	1.00*	1.00	2.25	2.25
SAFTMOD Output	0	0.80	1.00	7.00	7.00

*Since no observation nodes were selected for VADOFT output, the VADOFT output file was the same size with echo levels 4 and 5.

Tables 4-4 and 4-5 are useful guides, but the relative execution times and file sizes will change as a function of selected options (e.g., Monte Carlo) and the time period being simulated. As an example, the size of the output echo file is not much larger with an echo level of 5 than with an echo level of 0 (see Table 4-5). This results from the input data echoes of the PRZM, VADOFT, and SAFTMOD modules always appearing in the output echo file. These input echoes are a relatively large portion of what would appear in the output echo file from a relatively short simulation period (2 months).

4.2.1.6 Example Input File--

An example input file for the Execution Supervisor is presented in Figure 4-4. Note that in this example, some of the ANAME fields are indented. It is possible to put the label required for ANAME anywhere within the first 24 columns. If an MS-DOS-compatible computer is being used, lower-case characters can be used in defining the label. Embedded blanks in the label are significant. For example, if the label should be 'ENDRUN', a blank space between 'END' and 'RUN' would result in the code not recognizing the label.

Note also that in this example VADOFT is OFF, but the input and output files are still declared in the files section of the input file. These lines will be ignored by the code. In general, the records within the options records section, file records section, and global parameter records section can be in any order. The one exception is that the number of chemicals must be defined before the parent species of those chemicals.

4.2.2 PRZM Input

This section will describe the development of data input files for PRZM. Brief descriptions of each parameter are included in the input format guidance in this section. A more detailed discussion that will aid the user in assigning values to specific input parameters is found in Section 5.

4.2.2.1 Meteorological File--
Information for one day only is included in each record of the meteorological file. An example of the read statement and record format appears below:

```
READ(FLMT,1000,END=999) MM, MD, MY, PRECIP, PEVP, TEMP, WIND, SOLRAD

1000 FORMAT (1X, 3I2, 5F10.0)

(1234567890123456789012345678901234567890123456789) [COLUMN NUMBER]

  010179       1.50      0.340       17.2                  [Example Record]
```

The format identifier, 3I2, indicates that there are six spaces (columns) for designating the month (MM), day (MD), and year (MY) of the meteorological data. The example 010179 indicates month 01, day 01, and year 1979. The 3F10.0 indicates that precipitation, (PRECIP), potentral evaporation, (PEVP), and temperature (TEMP) are to be found in three separate blocks consisting of 10 columns each. PEVP and TEMP are not always required together; various combinations are possible depending on the observed data or climate (i.e., geographical areas in which snow accumulation and melting should be simulated will require temperature data). Wind speed and solar radiation data are required when the options to simulate volatilization and soil temperature are selected.

4.2.2.2 PRZM Parameter File--
Each line (representing a record) in the parameter file has a specified number of parameters in it. Each line has a formatted designation and is right justified. The user should make sure that the parameters for each line (record) required for a specific run has a value specified so that the READ statement will not go to the next line searching for a parameter file value (this will probably initiate an error message). Each line and the input data parameters for each line are discussed below (in the order required by the model). Sample PRZM input files are shown in Figures 6.4 and 6.7.

<u>RECORD 1</u>. TITLE

FORMAT (20A4)

TITLE(10): A specific title is developed for the simulation which appears in output files, e.g., Calibration Run Albany, Georgia. A total of 80 characters can be input to the title record.

<u>RECORD 2</u>. HTITLE

FORMAT (20A4)

HTITLE(10): This record provides a comment line of 80 characters for the user to input information regarding hydrology parameters.

RECORD 3. PFAC, SFAC, IPEIND, ANETD, INICRP, ISCOND

FORMAT (2F8.0, I8, F8.0, 2I8)

PFAC: Pan factor, dimensionless. This factor is multiplied by daily pan evaporation to estimate daily evapotranspiration (ET). If daily air temperatures are used for ET, any number can be input for PFAC (e.g., 0.75).

SFAC: Snow factor, cm-snowmelt/°C above freezing. Values of snow factor are in the order of 0.45. If snowmelt is not to be calculated, enter 0.00 for SFAC.

IPEIND: Pan evaporation flag. If IPEIND = 0, pan evaporation data are read. If IPEIND = 1, temperature data are read and used to calculate potential ET. If IPEIND = 2, then pan evaporation, if available, is used in the meteorologic file; if not, temperature is used to compute potential ET.

ANETD: Minimum depth, cm, to which evaporation is extracted year round (e.g., 20.0).

INICRP: User specified initial crop number if simulation starting date is before first crop emergence date (see record 8).

ISCOND: User specified surface condition after harvest corresponding to INICRP (either fallow, cropping, or residue, corresponding to dimensionless integer of 1, 2 or 3).

RECORD 3A. DT (Only if IPEIND = 1 or 2; DO NOT include this record if IPEIND = 0)

FORMAT (6F8.0)

DT(12): Average daily hours of daylight for each month. A total of 12 values (one for each month) are input using two lines in the parameter file.

RECORD 4. ERFLAG

FORMAT (I8)

ERFLAG: Erosion flag. If erosion losses are not to be calculated, ERFLAG = 0, otherwise ERFLAG = 1.

RECORD 4A. USLEK, USLELS, USLEP, AFIELD, TR (Only if ERFLAG = 1; DO NOT include this record if ERFLAG = 0).

FORMAT (5F8.0)

USLEK: Universal soil loss equation (K) soil erodibility parameter (e.g., 0.15).

USLELS: Universal soil loss equation (LS) topographic factor (e.g., 0.14).

USLEP: Universal soil loss equation (P) supporting practice factor (e.g., 1.0).

AFIELD: Area of field or plot (ha).

TR: Average duration of rainfall from runoff producing storms (hrs).

RECORD 5. NDC

FORMAT (I8)

NDC: Number of different crops used in the simulation (minimum of 1).

RECORD 6. ICNCN, CINTCP, AMXDR, COVMAX, ICNAH, CN, USLEC, WFMAX, HTMAX

FORMAT (I8, 3F8.0, I8, 3(1X, I3), 3(1X, F3.0), 2F8.0)

NOTE: This record must be repeated for each of the crops (NDC).

ICNCN: Crop number.

CINTCP: Maximum interception storage of the crop (cm).

AMXDR: Maximum active root depth of the crop (cm).

COVMAX: Maximum areal coverage of the crop at full canopy (percent).

ICNAH: Soil surface condition after crop harvest (1 = fallow, 2 = cropping, 3 = residue).

CN: Runoff curve number for antecedent soil water condition II, for fallow, crop, and residue fractions of the growing season (e.g. 86, 78, 82).

USLEC: Universal soil loss equation cover management factor. Three values must be entered in the same order as (CN), fallow, crop, and residue. Values only are required if ERFLAG = 1. Leaving them in the input file will have no effect if ERFLAG = 0 (e.g., 0.20).

WFMAX: Maximum dry foliage weight of the crop at full canopy kg m^{-2}. Only required if the exponential filtration model is used for pesticide application (values of WFMAX will not affect the simulation if FAM = 1 or 2, see record 12).

HTMAX: Maximum height of crop canopy at maturity (cm). Only used when simulating volatilization. Otherwise, it should be set to zero.

RECORD 7. NCPDS

FORMAT (I8)

NCPDS: Number of cropping periods in the simulation (minimum of 1). If three cropping years of continuous corn are simulated, NCPDS = 3. If two winter cover crops are in the middle of the three years of corn, NCPDS = 5.

RECORD 8. EMD, EMM, IYREM, MAD, MAM, IYRMAT, HAD, HAM, IYRHAR, INCROP

FORMAT (2X, 3I2, 2X, 3I2, 2X, 3I2, I8)

NOTE: This record must be repeated for each cropping period (NCPDS).

EMD: Day of month of crop emergence (e.g., 20).

EMM: Month of crop emergence (e.g., 4).

IYREM: Year of crop emergence (e.g., 82).

MAD: Day of month of crop maturation (e.g., 15).

MAM: Month of crop maturation (e.g., 10).

IYRMAT: Year of crop maturation (e.g., 82).

HAD: Day of month of crop harvest (e.g., 20).

HAM: Month of crop harvest (e.g., 10).

IYRHAR: Year of crop harvest (e.g., 82).

INCROP: Crop number of crop growing in current period (e.g., 1).

RECORD 9. PTITLE

FORMAT (20A4)

PTITLE(10): This record provides a comment line of 80 characters for the user to input information regarding pesticide parameters.

RECORD 10. NAPS, NCHEM

FORMAT (10I8)

NAPS: Number of pesticide applications (minimum of 1).

NCHEM: Number of different chemicals being simulated (minimum of 1).

RECORD 10A. PSTNAM

FORMAT (3A20)

PSTNAM: Name of pesticide. Up to three can be entered in the sequence in which they are to be simulated.

RECORD 11. APD, APM, IAPYR, DEPI, TAPP

FORMAT (2X, 3I2, 2F8.0)

NOTE: This record should be repeated for each application up to the total number of applications (NAPS).

APD: Day of the month of pesticide application (e.g., 10).

APM: Month of pesticide application (e.g., 5).

IAPYR: Year of pesticide application (e.g., 82).

DEPI: Depth of pesticide incorporation (cm).

TAPP: Total pesticide application (kg ha^{-1}). An application rate is required for each chemical in the sequence in which they are to be simulated.

RECORD 12. FAM, IPSCND, FILTRA

FORMAT (2I8, F8.0)

FAM: Pesticide application model. There are three options: FAM = 1 indicates application to soil only, FAM = 2 indicates a foliar application using a linear model (based on the percent of areal coverage by crop) and FAM = 3 indicates a foliar application using the exponential filtration model.

IPSCND: User-specified condition for disposition of pesticide remaining on foliage after harvest (either surface-applied, complete removal, or pesticide remains in plant compartment, conditions corresponding to integers 1, 2, or 3).

FILTRA: Filtration parameter for exponential model (only required if FAM = 3).

RECORD 12A. PLVKRT, PLDKRT, FEXTRC (only if FAM = 2 or 3; DO NOT include this record if FAM = 1). This record must be repeated NCHEM times.

FORMAT (3F8.0)

PLVKRT: Pesticide volatilization rate from plant foliage (day^{-1}).

PLDKRT: Pesticide decay rate on plant foliage (day^{-1}).

FEXTRC: Foliar extraction coefficient for pesticide washoff per centimeter of precipitation (e.g., 0.10).

RECORD 13. STITLE

FORMAT (20A4)

STITLE(10): This record provides a comment line of 80 characters for the user to input information regarding soils properties.

RECORD 14. CORED, UPTKF, BDFLAG, THFLAG, KDFLAG, HSWZT, MCFLAG, IRFLAG, ITFLAG, IDFLAG

FORMAT (2F8.0, 8I4)

CORED: Total depth of soil core (cm).

UPTKF: Plant uptake efficiency factor; UPTKF = 0 indicates no plant uptake simulated, UPTKF = 1 indicates uptake is simulated and is equal to the normalized crop transpiration rate times the dissolved phase concentration, 0<UPTKF<1 (e.g., 0.10) indicates uptake is simulated and is a fraction of the normalized crop transpiration rate times the dissolved phase concentration.

BDFLAG: Bulk density flag; BDFLAG = 0 indicates apparent bulk density known and entered (see RECORD 18A), BDFLAG = 1 indicates apparent bulk density to be calculated and mineral bulk density entered (see RECORD 18A).

THFLAG: Calculation flag for soil field capacity and wilting point water contents; THFLAG = 0 indicates water contents are entered (see RECORD 18), THFLAG = 1 indicates water contents will be calculated by the model.

KDFLAG: Calculation flag for soil/pesticide adsorption partition coefficients; KDFLAG = 0 indicates partition coefficients are entered (see 19), KDFLAG = 1 indicates partition coefficients will be calculated by the model.

HSWZT: Switch for soil hydraulics; HSWZT = 0 indicates free-draining soils, HSWZT = 1 indicates restricted-drainage soils.

MCFLAG: Flag for running the MOC algorithm; MCFLAG = 0 if MOC is not used, MCFLAG = 1 if MOC is used.

IRFLAG: Flag for irrigation simulation; IRFLAG = 0 for no irrigation; IRFLAG = 1 if irrigation is simulated.

ITFLAG: Soil temperature simulation; ITFLAG = 0 for no temperature simulation; ITFLAG = 1 if soil temperature is simulated. The only reason to simulate soil temperature is to correct Henry's constant for temperature effects. Therefore, unless chemical volatilization is being simulated, soil temperature simulation should be suppressed.

IDFLAG: Thermal conductivity and heat capacity flag; IDFLAG = 0 if values are to be entered, IDGLAG = 1 if values are to be calculated by the model. These calculations are only required to support soil temperature calculations.

RECORD 15. DAIR, HENRYK, ENPY

FORMAT (F8.0, 3(2F8.0))

DAIR: Diffusion coefficient (cm^2 day^{-1}) for the pesticide in air (one value). Only required if HENRYK > 0.

HENRYK: Henry's Law constant for each of the NCHEM pesticides.

ENPY: Enthalpy of vaporization (kcal mole^{-1}) for each of the NCHEM pesticides. Only required if ITFLAG = 1 and HENRYK > 0. ENPY = 0 indicates no temperature correction for Henry's Constant.

RECORD 15.1 IRTYPE, FLEACH, PCDEPL, RATEAP (Only if IRFLAG = 1)

FORMAT (I5, 3F8.0)

IRTYPE: Irrigation flag which determines the type of irrigation modeled by PRZM.

IF IRTYPE = 0, no irrigation water is applied
= 1, flood irrigation
= 2, furrow irrigation
= 3, over-canopy sprinkler irrigation
= 4, under-canopy sprinkler irrigation.

FLEACH: Leaching factor, as fraction of irrigation water depth. FLEACH allows extra water to be added for leaching of salts from saline soils.

PCDEPL: Fraction of the available water capacity at which irrigation is triggered. If the average root zone soil moisture level falls below PCDEPL, irrigation water is applied.

RATEAP: Maximum rate of water sprinklers can deliver, cm^{-1} hr. This variable is required only if sprinkler irrigation is used (IRTYPE = 3,4).

RECORD 15.1A Q0, BT, Z, SF, EN, XL, XFRAC (Included only for furrow irrigation, IRTYPE = 2 and IRFLAG = 1)

FORMAT (7F8.0)

Q0: Flow rate of water entering the heads of individual furrow ($m^3 s^{-1}$).

BT: Bottom width of furrows (m).

Z: Slope of furrow channel side walls (horizontal/vertical).

SF: Slope of furrow channel bottom (vertical/horizontal).

EN: Manning's roughness coefficient for the furrow.

XL: Length of the furrow (m).

XFRAC: Location in furrow where PRZM infiltration calculations are performed, as fraction of the furrow length XL. IF XFRAC = -1, average furrow infiltration depths are used in PRZM.

RECORD 15.1B KS, HF (included only for furrow irrigation, IRTYPE = 2 and IRFLAG = 1)

FORMAT (2F8.0)

KS: Saturated hydraulic conductivity of soil in which furrows are dug (m/s).

HF: Green-Ampt infiltration suction parameter (m).

RECORD 16A. PCMC, SOL (Only if KDFLAG = 1, DO NOT include if KDFLAG = 0)

FORMAT (I8, F8.0)

PCMC: Calculation flag for model to estimate pesticide soil partition coefficients. There are three options: PCMC = 1, PCMC = 2, and PCMC = 3.

SOL: Pesticide solubility. The units vary according to the model (PCMC) selected; PCMC = 1, mole fraction; PCMC = 2, mg $liter^{-1}$; PCMC = 3, micromoles $liter^{-1}$.

RECORD 16B. ALBEDO, EMISS, ZWIND (Only if ITFLAG = 1, do not include if ITFLAG = 0)

FORMAT (14F5.0)

ALBEDO(12): Monthly values of soil surface albedo (fraction).

EMISS: Reflectivity of the soil surface to longwave radiation (fraction).

ZWIND: Height of wind speed measurement (m) above soil surface.

RECORD 16C. BBT (Only if ITFLAG = 1, do not include if ITFLAG = 0)

FORMAT (12F5.0)

BBT(12): Average monthly values of bottom boundary soil temperatures (^{o}C).

RECORD 17. NHORIZ

FORMAT (I8)

NHORIZ: Total number of soil horizons (minimum of 1).

NOTE: Records 18A through 22 are read in (as required) for each soil horizon up to number of horizons (NHORIZ) input. The specific records read depend on the values of flags set on record 14.

RECORD 18A. HORIZN, THKNS, BD, THETO, DISP, DWRATE, DSRATE, DGRATE (Include only if HSWZT = 0)

FORMAT (I8, 3F8.0, 16X, 4F8.0)

HORIZN: Soil horizon number.

THKNS: Soil horizon thickness (cm).

BD: Soil bulk density (if BDFLAG = 0) and/or mineral bulk density (if BDFLAG = 1).

THETO: Initial soil water content in the horizon (cm^3 cm^{-3}).

DISP: Hydrodynamic solute dispersion coefficient (cm^2 day^{-1}) (only required here if NCHEM = 1).

DWRATE: Dissolved phase pesticide decay rate in the horizon (day^{-1}) (only required here if NCHEM = 1).

DSRATE: Adsorbed phase pesticide decay rate in the soil horizon (day^{-1}) (only required here if NCHEM = 1).

DGRATE: Vapor phase pesticide decay rate in the soil horizon (day^{-1}) (only required here if NCHEM = 1).

RECORD 18B. HORIZN, THKNS, BD, THETO, AD, DISP, DWRATE, DSRATE, DGRATE (Include only if HSWZT = 1)

FORMAT (I8, 4F8.0, 8X, 4F8.0))

HORIZN: See record 18A.
THKNS: See record 18A.
BD: See record 18A.
THETO: See record 18A.
AD: Soil horizon drainage parameter (day^{-1}). Used only if HSWZT = 1, otherwise the value is ignored.
DISP: See record 18A.
DWRATE: See record 18A.
DSRATE: See record 18A.
DGRATE: See record 18A.

RECORD 19A. DPN, THEFC, THEWP, KD (Only if THFLAG = 0, BDFLAG = 0, and KDFLAG = 0)

FORMAT (8X, 3F8.0, 8X, F8.0)

DPN: Soil layer depth in soil horizon.

THEFC: Field capacity soil water content in horizon ($\text{cm}^3\ \text{cm}^{-3}$).

THEWP: Wilting point soil water content in horizon ($\text{cm}^3\ \text{cm}^{-3}$).

KD: Sorption partition coefficient for soil horizon/pesticide combination ($\text{cm}^3\ \text{g}^{-1}$) (only required here if NCHEM = 1).

RECORD 19B. DPN, THEFC, THEWP, OC, KD (Only if KDFLAG = 0, THFLAG = 0 and BDFLAG = 1)

FORMAT (8X, 5F8.0)

DPN: See record 19A.
THEFC: See record 19A.
THEWP: See record 19A.
OC: Organic carbon content of the soil horizon (percent).
KD: See record 19A.

RECORD 19C. DPN, THEFC, THEWP, OC (Only if THFLAG = 0 and KDFLAG = 1)

FORMAT (8X, 4F8.0)

DPN: See record 19A.
THEFC: See record 19A.
THEWP: See record 19A.
OC: Organic carbon content of soil horizon (percent). This value is also required if BDFLAG = 1.

RECORD 19D. DPN, SAND, CLAY, OC, KD (Only if THFLAG = 1 and KDFLAG = 0)

FORMAT (8X, 5F8.0)

DPN: See record 19A.
SAND: Percent sand in soil horizon.
CLAY: Percent clay in soil horizon.
OC: Organic carbon content of soil horizon (percent). This value is also required if BDFLAG = 1.
KD: Sorption partition coefficient for soil horizon/pesticide combination ($cm^3\ g^{-1}$) (only required here if NCHEM = 1).

RECORD 19E. DPN, SAND, CLAY, OC (Only if THFLAG = 1 and KDFLAG = 1)

FORMAT (8X, 4F8.0)

DPN: See record 19A.

SAND: Percent sand in soil horizon.

CLAY: Percent clay in soil horizon.

OC: Organic carbon content of soil horizon (percent). This value is also required if BDFLAG = 1.

RECORD 20A. SPT, SAND, CLAY, OC (Only if ITFLAG = 1, IDFLAG = 1, and THFLAG = 0)

FORMAT (8X, 4F8.0)

SPT: Initial temperature of soil horizon (^oC).

SAND: See record 19D.

CLAY: See record 19D.

OC: See record 19C.

RECORD 20B. SPT (Only if ITFLAG = 1, IDFLAG = 1 and THFLAG = 1)

FORMAT (8x, F8.0)

SPT: See record 20A.

RECORD 20C. SPT, THCOND, VHTCAP (Only if ITFLAG = 1 and IDFLAG = 0)

FORMAT (8X, 3F8.0)

SPT: See record 20A.

THCOND: Thermal conductivity of soil horizon ($cal\ cm^{-1}\ day^{-1}\ ^oC^{-1}$).

VHTCAP: Heat capacity per unit volume of soil horizon (cal cm^{-3} $^{o}C^{-1}$).

RECORD 21A. DWRATE, DSRATE, DGRATE, KD, DISP (Record 21A is repeated for each chemical for the horizon, only required if NCHEM > 1).

FORMAT (8X, 5F8.0)

DWRATE: See record 18A.

DSRATE: See record 18A.

DGRATE: See record 18A.

KD: See record 18A.

DISP: See record 18A.

RECORD 22. DKRT12, DKRT13, DKRT23 (Record 22 is only required if NCHEM > 1)

FORMAT (8X, 3F8.0)

DKRT12: Transformation rate from pesticide 1 to 2 (day^{-1}).

DKRT13: Transformation rate from pesticide 1 to 3 (day^{-1}).

DKRT23: Transformation rate from pesticide 2 to 3 (day^{-1}).

RECORD 23. ILP, CFLAG

FORMAT (2I8)

ILP: Initial level of pesticide indicator. Signals user to input an initial pesticide storage. ILP = 0, indicates no initial levels input; ILP = 1, indicates initial levels are being input.

CFLAG: Conversion flag for initial pesticide level input. CFLAG=0, indicates input in mg kg^{-1}; CFLAG = 1, indicates input in kg ha^{-1}. This flag need not be assigned if ILP = 0.

RECORD 23A. PESTR (Only if ILP = 1)

FORMAT (8F8.0)

PESTR: Initial pesticide level in each compartment (up to NCOM2) for each chemical. Note that the user must calculate the total number of compartments by using the thickness of each horizon and its associated compartment thickness. Enter NCOM2/8 lines of data for each chemical. Repeat for each chemical. Input must be either in mg kg^{-1} or kg ha^{-1}.

RECORD 24. ITEM1, STEP1, LFREQ1, ITEM2, STEP2, LFREQ2, ITEM3, STEP3, LFREQ3

FORMAT (3(4X, A4, 4X, A4, I8))

NOTE: For hard copy output.

ITEM1: Hydrologic output summary indicator. WATR is inserted to call hydrologic summaries. A blank is left for ITEM1 if hydrologic summaries are not desired.

STEP1: Time step of output. Three options are available: DAY for daily, MNTH for monthly, or YEAR for annual output.

LFREQ1: Frequency of soil compartment reporting. Example: LFREQ1 = 1, every compartment is output; LFREQ = 5, every fifth compartment is output.

ITEM2: Pesticide output summary indicator. PEST is inserted to call pesticide mass summaries. A blank is inserted for ITEM2 if pesticide summaries are not desired.

STEP2: Same as STEP1.

LFREQ2: Same as LFREQ1.

ITEM3: Pesticide concentration profile indicator. CONC is inserted to call pesticide concentration profile summaries. A blank is inserted if concentration profiles are not desired.

STEP3: Same as STEP1.

LFREQ3: Same as LFREQ1.

RECORD 25. NPLOTS, STEP4

FORMAT (I8, 4X, A4)

NPLOTS: Number of time series plots to be output (maximum of 7)

STEP4: Time step of output. This option outputs pesticide runoff flux, pesticide erosion flux and pesticide leaching below core depth to a single output data file for later use. Three options are available: DAY for daily, MNTH for monthly, or YEAR for annual output.

RECORD 25A. PLNAME, INDX, MODE, IARG, CONST, (Only if NPLOTS > 0) (Repeat record for each time series output)

FORMAT (4X, A4, A1, 3X, A4, I8, F8.0, 7X, A1, I8)

PLNAME: Name of time series. Possible options are listed in Table 4-6.

INDX: Index to identify pesticide; INDX values of 1, 2, 3 indicate pesticide 1, 2, or 3. Leave blank if other timeseries are plotted.

MODE: Plotting mode. Two options are available: TSER provides the time series as output, TCUM provides the cumulative time series.

IARG: Argument of variable identified in PLNAME. Example: INFL is specified which corresponds to AINF within the FORTRAN program. AINF is dimensioned from 1 to NCOM2. IARG must be specified to identify the soil compartment (1 to NCOM2) reporting for AINF (IARG is left blank for scalers).

CONST: Specifies a constant with which the user can multiply the times series for unit conversion, etc. If left blank a default of 1.0 is used.

RECORD 26. ATITLE

FORMAT (20A4)

ATITLE: Title for special action.

RECORD 27. SADAY, SAMON, SAYR, SPACT, NACTS, SPACTS

FORMAT (2X, 3I2, 1X, 2A4, 1X, I3, 3F8.0)

SADAY: Day of month of special action.

SAMON: Month of special action.

SAYR: Year of special action.

SPACT: Variable affected by special action.

NACTS: Horizon or crop numbers affected by special action.

SPACTS: New value(s) for the special action. Possible values for NACTS and SPACTS are listed below:

SPACT (2A4)	NACTS (I3)	SPACTS (3F8.0)
BD	Horizon no.	New value
CN	Crop no.	New values (3)
DSRATE	Horizon no.	New values (3)
DWRATE	Horizon no.	New values (3)
KD	Horizon no.	New values (3)
SNAPSHOT*	---	---
USLEC	Crop no.	New values (3)

* Display pesticide concentration profile

Table 4-6. VARIABLE DESIGNATIONS FOR PLOTTING FILES

Variable Designation (PLNAME)	FORTRAN Variable	Description	Units	Arguments Required (IARG)
Water Storage				
INTS	CINT	Interception storage on canopy	cm	None
SWTR	SW	Soil water storage	cm	1-NCOM2
SNOP	SNOW	Snow pack storage	cm	None
THET	THETN	Soil water content	cm cm^{-1}	1-NCOM2
Water Fluxes				
PRCP	PRECIP	Precipitation	cm day^{-1}	None
SNOF	SNOWFL	Snowfall	cm day^{-1}	None
THRF	THRUFL	Canopy throughfall	cm day^{-1}	None
INFL	AINF	Percolation into each soil compartment	cm day^{-1}	1-NCOM2
RUNF	RUNOF	Runoff depth	cm day^{-1}	None
CEVP	CEVAP	Canopy evaporation	cm day^{-1}	None
SLET	ET	Actual evapotranspiration from each compartment	cm day^{-1}	1-NCOM2
TETD	TDET	Total daily actual evapotranspiration	cm day^{-1}	None
Sediment Flux				
ESLS	SEDL	Event soil loss	Tonnes day^{-1}	None
Pesticide Storages				
FPST	FOLPST	Foliar pesticide storage	g cm^{-2}	None

Table 4-6. VARIABLE DESIGNATIONS FOR PLOTTING FILES (continued)

Variable Designation (PLNAME)	FORTRAN Variable	Description	Units	Arguments Required (IARG)
Pesticides Storages				
TPST	PESTR	Total soil pesticide storage in each soil compartment	g cm^{-3}	1-NCOM2
SPST	SPESTR	Dissolved pesticide storage in each soil compartment	g cm^{-3}	1-NCOM2
Pesticide Fluxes				
TPAP	TAPP	Total pesticide application	g cm^{-2} day^{-1}	None
FPDL	FPDLOS	Foliar pesticide decay loss	g cm^{-2} day^{-1}	None
WFLX	WOFLUX	Foliar pesticide washoff flux	g cm^{-2} day^{-1}	None
DFLX	DFFLUX	Individual soil compartment pesticide net diffusive flux	g cm^{-2} day^{-1}	1-NCOM2
AFLX	ADFLUX	Pesticide advective flux from each soil compartment	g cm^{-2} day^{-1}	1-NCOM2
DKFX	DKFLUX	Pesticide decay flux in each soil compartment	g cm^{-2} day^{-1}	1-NCOM2
UFLX	UPFLUX	Pesticide uptake flux from each soil compartment	g cm^{-2} day^{-1}	1-NCOM2
RFLX	ROFLUX	Pesticide runoff flux	g cm^{-2} day^{-1}	None
EFLX	ERFLUX	Pesticide erosion flux	g cm^{-2} day^{-1}	None

Table 4-6. VARIABLE DESIGNATIONS FOR PLOTTING FILES (concluded)

Variable Designation (PLNAME)	FORTRAN Variable	Description	Units	Arguments Required (IARG)
Pesticide Fluxes				
RZFX	RZFLUX	Net pesticide flux past the maximum root depth	$g\ cm^{-2}\ day^{-1}$	None
TUPX	SUPFLX	Total pesticide uptake flux from entire soil profile	$g\ cm^{-2}\ day^{-1}$	None
TDKF	SDKFLX	Total pesticide decay flux from entire profile	$g\ cm^{-2}\ day^{-1}$	None
PCNC	TCNC	Pesticide concentration in canopy	$g\ cm^{-3}$	None
VFLX	PVFLUX	Soil pesticide volatilization flux	$g\ cm^{-2}\ day^{-1}$	None
FPVL	FPVLOS	Foliar pesticide volatilization flux	$g\ cm^{-2}\ day^{-1}$	None
Soil Temperature				
STMP	SPT	Soil temperature in each soil compartment	°C	1-NCOM2
Canopy Height				
CHGT	HEIGHT	Canopy height	cm	None

4.2.3 VADOFT Input

VADOFT is designed to run one flow and/or a flow and associated transport problem when run in the linked mode. When running both flow and transport, the flow and transport input data are stacked in the same input file. An example input file is shown in Section 6. Figure 6.8 shows the flow portion of the file and Figure 6.9 shows the transport portion.

An option is provided in VADOFT for automatic generation of Default initial values. This option is invoked by setting the input variables NONU and NPIN equal to zero. When this is the case, all nodal values of the dependent variable (head or concentration) will be set equal to the default initial value.

Any set of consistent units for physical parameters may be used for VADOFT input. However, when run in the linked mode, length units should be cm and time units in days. To facilitate data entry, the input data is divided into 15 groups, arranged as follows:

1. Title record
2. Control records
3. Input/output control record
4. Time discretization record
5. Spatial discretization data
6. Default initial and boundary condition record
7. Boundary condition record
8. Saturated material property records
9. Soil moisture data records
10. Initial condition records
11. Solute transport parameter records
12. Velocity input file control record
13. Time-dependent boundary condition records for node 1
14. Time-dependent boundary condition records for node NP
15. Observation node records.

This sequence must be strictly followed when entering data into the program. A description of the input variables and data formats follows.

Group 1. Title record (A80)

One record.

Col. 1-80 TITLE: Title of problem.

Group 2. Control records

(a) Simulation control record (11I5)

One record.

Col. 1-5 NP: Total number of nodal points in the selected grid.

6-10	NTS:	Total number of time steps. For a steady-state simulation, the code automatically sets NTS = 1. (Note that steady-state simulation is not allowed when running in the linked mode. See the ITRANS parameter, this group.) When running in the linked mode, NTS is a dummy input. The value input here is overridden with a value (NLDLT) from the execution supervisor.
11-15	NMAT:	Number of different porous materials.
16-20	NONU:	Parameter indicating if the initial condition is nonuniform; = 0 if no, = 1 if yes and data is read from the input file.
21-25	ITRANS:	Parameter indicating if the simulation is to be performed in a transient mode. Currently, the program will stop if PRZM is being run with VADOFT and ITRANS is not set to 1 here. = 1 if yes, = 0 if no.
26-30	IMODL:	Parameter indicating the type of simulation. Note that when running a coupled flow and transport simulation, the flow simulation input must be first in the input file. = 1 for water flow. = 0 for solute transport.
31-35	IKALL:	Time stepping index; = 1 for backward difference scheme, = 0 for central difference scheme. For a steady-state simulation, the code automatically uses the backward difference scheme.
36-40	IMBAL:	Parameter indicating if mass balance computation is required. This must be set to 1 in order for mass balance information to be output. = 1 if yes, = 0 if no.

*** If performing the transport simulation, leave columns 41-45 blank.

41-45	INTSPC:	Parameter specifying if the initial condition for the flow simulation is in terms of pressure head or hydraulic head;

= 1 for hydraulic head specification,
= 0 for pressure head specification.

46-50 IHORIZ: Parameter indicating if the flow direction is horizontal; this should always be set to 0 for linked model applications;
= 1 if yes,
= 0 if no.

51-55 ICHAIN: Parameter indicating if the simulation involves simulation of daughter products;
= 1 if yes,
= 0 if no.
In the case of flow simulation, the code automatically sets ICHAIN to zero.

(b) Iteration control record (3I5, E10.3)

*** Omit if performing transport simulation.

One record.

Col. 1-5 NITMAX: Maximum number of nonlinear iterations allowed per time step.

6-10 INEWT: Parameter indicating the type of nonlinear iterative procedure to be used in solving the variably saturated flow equation;
= 0 for Picard procedure,
= 1 for standard Newton-Raphson procedure,
= 2 for modified Newton-Raphson procedure.
The use of modified Newton-Raphson procedure is recommended for cases of highly nonlinear soil moisture curves and when running VADOFT in the linked mode with PRZM.

1-15 IRESOL: Maximum number of refinements of time steps allowed if the solution of the variably saturated flow equation does not converge. Suggested value of IRESOL = 1.

16-25 HTOL: Head tolerance to be used in the nonlinear solution. As a guide, the value of HTOL should be set to (a/100)*(difference between expected maximum and minimum head values) for a% accuracy. The absolute limit of a is 10^{-5} for single precision and 10^{-12} for double precision.

Group 3. Input/output control record (8I5)

One record.

Col. 1-5	KPROP:	Parameter indicating the type of relationships of relative permeability versus saturation, and pressure head versus saturation; = 1 if functional parameters are to be supplied, = 0 if tabulated values are to be supplied. Set KPROP = 0 for a fully saturated flow or a transport analysis.
6-10	ITSGN:	Parameter indicating if time values are to be generated; = 1 if yes, = 0 if no. For linked mode operation, it is most convenient to set ITSGN to 1. For a steady-state simulation, the code automatically sets ITSGN = 1.
11-15	ITMARK:	Parameter indicating if marker time values at which output is to be written on backup files differ from computational time values. This parameter should be set to 1 when running in the linked mode. = 1 if yes, = 0 if no.
16-20	NSTEP:	Parameter controlling printout of computed nodal values. When NSTEP = n, results are printed for each nth time step. Note that when running in linked mode, this is a dummy input. Printing frequency of flow and transport output is controlled by the water and pesticide reporting frequency specified in PRZM.
21-25	NVPR:	Parameter controlling printout of velocities. Set NVPR = n if nodal velocities are to be printed for each nth time step. When running in linked mode, this is a dummy input. Nodal velocities are written to the file at the end of each marker time value (i.e., each day).
26-30	IOBSND:	Parameter indicating if values at some specified observation nodes are to be recorded for all time steps; = 1 if yes, = 0 if no.

31-35	NOBSND:	Number of observation nodes. Leave blank or set = 0, if IOBSND = 0.
36-40	IPRCHK:	Print check parameter; = 1 if printcheck is required, = 0 if no printcheck is required. If IPRCHK is set to 1, detailed information utilized in the flow and transport matrix assembly routines is printed.

Group 4. Temporal data

*** Omit if performing steady-state simulation (ITRANS=0).

(a) Time parameters (4E10.3)

If ITSGN = 0, leave Cols. 11-40 blank.

One record.

Col. 1-10	TIMA:	Initial time value. For running in linked mode, this should be set to 0.0
11-20	TIN:	Initial time step value. For linked mode operation, should be set to 1.0.
21-30	TFAC:	Time-step multiplier. For linked mode operation, should be set to 1.0.
31-40	TMAX:	Maximum value of time step allowed. For linked mode operation, should be set to 1.0.

(b) Computational time values (8E10.3)

*** Omit if ITSGN = 1.

Number of records = NTS/8 + 0 or 1.

Col. 1-10 11-20 etc.	TMVEC(I):	Time values, where I = 1,...., NTS.

Note: TMVEC(1) must be greater than zero, and TMVEC(1) through TMVEC(NTS) must be in sequential order of increasing value.

(c) Output marker time data

*** Omit if ITMARK = 0.

First record (2I5,2E10.3)

Col. 1-5 NTOMT: Number of backup file output maker time values. For linked mode operation, this should be set to the number of days in a SAFTMOD timestep (i.e., same value as NLDLT in the Execution Supervisor input).

6-10 ITMGEN: Parameter indicating if marker time values are to be generated by the code;
= 1 if yes,
= 0 if no.
For linked mode operation, set ITMGEN to 1.

11-20 STMARK: Starting marker time value. For linked mode operation set STMARK to -0.01.

21-30 DTMARK: Marker time increment. If ITMGEN = 0, omit Cols. 11-30. For linked mode operation, set DTMARK equal to 1.0.

Remaining records (8E10.3)

*** Omit if ITMGEN = 1.

Number of records = NTOMT/8 + 0 or 1.

Col. 1-10 TMFOMT(I): Output marker time values for backup files, where I = 1,...., NTOMT.
11-20
etc.

Group 5. Spatial discretization data

(a) Control parameter (I5)

Col. 1-5 NLAYRG: Number of layers (horizons) that need to be discretized.

(b) Grid layer data (3I5,E10.3)

Number of records - NLAYRG.

Col. 1-5 ILAYR: Layer number.

6-10 NELM(ILAYR): Number of finite elements in layer ILAYR.

11-15 IMATL(ILAYR): Material number of layer ILAYR.

16-26 THL(ILAYR): Thickness of layer ILAYR.

Group 6. Initial condition data (5(E10.3,I5))

One record.

Col. 1-10 HINV: Default initial value of head (or concentration). In the water flow simulation, the code allows HINV to be either the initial pressure head or the initial hydraulic head.

11-15 NPIN: Number of (nondefault) nodes where initial value differs from the default value. For multiple chemicals read in the values of HINV and NPIN for each chemical sequentially on this line.

Group 7. Boundary condition record (2I5,2E10.3,2I5,2E10.3)

One record.

Col. 1-5 IBTND1: Boundary condition type specification for the first node;
= 1 if pressure head (or concentration) is specified,
= 0 if water (or solute) flux is specified.
When run in linked mode (i.e., PRZM is ON) IBTND1 is automatically set to 0 in the code.

6-10 IBTNDN: Boundary condition type specification for the last node;
= 1 if pressure head (or concentration) is specified,
= 0 if water (or solute) flux is specified.
When run in linked mode (i.e., SAFTMOD is ON), IBTNDN is automatically set to 1.

11-20 VALND1: For a flow simulation, VALND1 denotes pressure head (if IBTND1 = 1) or water flux (if IBTND1 = 0) at node 1. For a transport simulation, VALND1 denotes concentration at node 1 (if IBTND1 = 1) or solute mass flux entering node 1 if (IBTND1 = 0). (The sign convention for the flux is: positive for influx and negative for efflux). This is a dummy input when operating in linked mode.

21-30 VALNDN: For a flow simulation, VALNDN denotes pressure head at node N (if IBTNDN = 1) or water flux at node N (if IBTNDN = 0). For a transport simulation, VALNDN denotes concentration at node 1 (if IBTNDN = 1). If the fluid is discharging or exiting at node NP, set VALNDN = 0 or leave blank. In linked mode, this is a dummy input; VALNDN is specified by SAFTMOD for flow and set to zero for transport automatically by the code.

31-35	ITCND1:	Parameter specifying if the boundary condition at node 1 is transient; = 1 if yes, = 0 if no. When running in linked mode, this is a dummy input. The code automatically sets ITCND1 to 0.
36-40	ITCNDN:	Parameter specifying if the boundary condition at node NP is transient; = 1 if yes, = 0 if no. When running in linked mode, this is a dummy input. The code automatically sets ITCNON to 0.
41-50	FLX1:	For a flow simulation, set FLX1 = 0. For a transport simulation, FLX1 is the value of fluid flux entering node 1. If the fluid is discharging or exiting at node 1, set FLX1 = 0, or leave blank. Not required for linked mode simulation (if PRZM is ON).
51-60	FLXN:	For a flow simulation, set FLXN = 0. For a transport simulation, FLXN is the value of fluid flux entering node NP. If the fluid is discharging or exiting at node NP, set FLXN = 0 or leave blank. Not required for linked mode simulation (if SAFTMOD is ON).

Group 8. Saturated material property records (8E10.3)

Number of records = NMAT.

*** If performing a flow simulation, specify the following information:

Col. 1-10	PROP(I,1):	Saturated hydraulic conductivity of material I.
11-20	PROP(I,2):	Effective porosity of material I.
21-30	PROP(I,3):	Specific storage of material I.
31-40	PROP(I,4):	Air entry pressure head value of material I.

*** If performing a transport simulation, specify the following information. Note that, for multiple chemicals, properties 3 and 4 are repeated for each chemical sequentially on this line (i.e., $(3,4)_{i=1}$, $(3,4)_{i=2}$, $(3,4)_{i=3}$):

Col. 1-10 PROP(I,1): Longitudinal dispersivity of material I.

11-20 PROP(I,2): Effective porosity of material I.

21-30 PROP(I,3): Retardation coefficient for chemical i in material I under fully saturated conditions ($R_{sat} = 1 + K_d\rho/\theta$).

31-40 PROP(I,4): Molecular diffusion coefficient for chemical i in material I.

Group 9. Soil moisture data records

(a) Functional coefficient values (5E10.3)

*** Omit if KPROP = 0 or if performing transport simulation (IMODL = 0).

Number of records = NMAT.

Col. 1-10 FVAL(I,1): Residual water phase saturation of (S_{wr}) of material number IMAT.

11-20 FVAL(I,2): Parameter (n) of the relative permeability versus saturation relationship. If n is greater than zero, the following relationship is used:

$$k_{rw} = S_e^n$$

where S_e is the effective saturation defined as

$$S_e = (S_w - S_{wr})/(1 - S_{wr}).$$

If n is less than or equal to zero, the following relationship is used:

$$k_{rw} = [1 - (1 - S_e{}^{1/\gamma})^\gamma]^2$$

where γ corresponds to FVAL(I,5).

21-30 FVAL(I,3): Leading coefficient (α) of the saturation versus capillary head relationship,

$$S_w - S_{wr} = (1 - S_{wr})/[1 + (\alpha|\psi - \psi_a|)^\beta]^\gamma.$$

31-40 FVAL(I,4): Power index (β) of the saturation versus capillary head relationship.

41-50 FVAL(I,5): Power index (γ) of the saturation versus capillary head relationship.

(b) Relative permeability versus saturation data

*** Omit if KPROP = 1 or if performing transport simulation (IMODL = 0).

Number of record sets = NMAT. Each set contains the following:

(i) Header record (I5)

Col. 1-5 NUMK(I): Number of entry pairs of relative permeability and saturation values for material I.

(ii) Data records (8E10.3)

Col. 1-10 SMV(I,1): Value of water phase saturation for data point 1 of material number I.

11-20 PKRW(I,1): Value of relative permeability at data point 1.

21-30 SMV(I,2): etc.

31-40 PKRW(I,2): etc.

(c) Pressure head versus saturation data

*** Omit if KPROP = 1 or if performing transport simulation (IMODL = 0).

Number of record sets = NMAT. Each set contains the following:

(i) Header record (I5)

Col. 1-5 NUMP(K): Number of entry pairs of pressure head versus saturation values for material I.

(ii) Data records (8E10.3)

Col. 1-10 SSWV(I,1): Value of water phase saturation for data point 1 of material number I.

11-20 HCAP(I,1): Value of pressure head for data point 1 of material number I.

21-30 SSWV(I,2): etc.

31-40 HCAP(I,2): etc.

Note: Values of water phase saturation must be arranged in increasing order.

Group 10. Initial condition records (5(I5,E10.3))

*** Omit if the initial condition is uniform (NONU = 0).

Number of records = NPIN/5 + 0 or 1. Nondefault initial conditions for multiple chemicals should be entered sequentially for each chemical (i.e., all nodes for chemical 1, all nodes for chemical 2, etc.). Begin reading nodes for each new chemical with a new record. For instance, if there are 3 nondefault nodes for chemical 1, and 3 for chemical 2, do not append the chemical 2 nondefault nodes to the end of the chemical 1 record, begin chemical 2 with a new record.

Col. 1-5 N: Node number.

6-15 etc. PINT(I): Nondefault initial value of head or concentration, where I = 1,...., NPIN.

Group 11. Solute transport parameter records (I5,4E10.3)

*** Omit if performing flow simulation (IMODL = 1).

(a) General data

Number of records = NMAT.

Col. 1-5 I: Porous material number.

6-15 VDFI(I): Default value of Darcy velocity for material I.

16-25 SWDFI(I): Default value of water saturation for material I.

26-35 DLAMDI(I): Value of decay constant of the solute for material I.

36-45 UWFI(I): Value of upstream weighting factor for material I. Set UWF = 0, if no upstream weighting is required.

(b) Transport parameter records (I5,6E10.3)

Number of records = 1 for each material.

Col. 1-5 I: Porous material number.

6-15 CLAMDI(I,1): Decay coefficient of chemical 1 in material I.

16-25	CRACMP(I,1):	Transformation mass fraction of chemical 1 in material I.
26-36	CLAMDI(I,2):	Decay coefficient of chemical 2 in material I. Omit if NCHEM is less than 2.
37-47	CRACMP(I,2):	Transformation mass fraction of chemical 2 in material I. Omit if NCHEM is less than 2.
48-58	CLAMDI(I,3):	Decay coefficient of chemical 3 in material I. Omit if NCHEM is less than 3.
59-69	CRACMP(I,3):	Transformation mass fraction of chemical 3 in material I. Omit if NCHEM is less than 3.

Group 12. Velocity input file control record (2I5)

*** Omit if performing flow simulation (IMODL = 1).

One record.

Col. 1-5	NVREAD:	Parameter indicating if velocities will be read from a scratch file. In linked mode, this parameter is reset to 1; = 1 if yes, = 0 if no.
6-10	IVSTED:	Parameter indicating if the velocity field is at a steady state. If PRZM is ON, this parameter will be reset to 1; (note: this implies that the velocity field is at steady-state within each day, not over the course of the simulation); = 1 if yes, = 0 if no.

Group 13. Time-dependent boundary condition records for node 1

*** Omit if ITCND1 = 0 or if PRZM is on.

If performing a water flow simulation, supply the following information:

(a) Control record (I5)

One record.

Col. 1-5	NTSNDH(1):	Number of selected time values on the time graph of pressure head (or water flux if IBTND1 = 0) at node 1.

(b) Time value records (8E10.3)

Number of records = NTSNDH(1)/8 + 0 or 1.

Col. 1-10 11-20 etc.	TMHV(1,J):	Time values at the selected interpolation points on the time graph of pressure head (or water flux if IBTND1 = 0) at node 1, where J = 1,...., NTSNDH(1).

(c) Functional value record (8E10.3)

Number of records = NTSNDH(1)/8 + 0 or 1.

Col. 1-10 11-20 etc.	HVTM(1,J):	Value of pressure head (or water flux if IBTND1 = 0) corresponding to TMHV(1,J), where J = 1,...., NTSNDH(1).

If performing solute transport simulation, supply the following information:

(a) Control record (I5)

One record.

Col. 1-15	NTSNDH(1):	Number of selected time values on the time graph of concentration (or solute flux if IBTND1 = 0).

(b) Time value records (8E10.3)

Number of records - NTSNDH(1)/8 + 0 or 1.

Col. 1-10 11-20 etc.	TMHV(1,J):	Time values at the selected interpolation points on the time graph of concentration (or solute flux if IBTND1 = 0) at node 1, where J = 1,..., NTSNDH(1).

(c) Functional value record (8E10.3)

Number of records = NTSNDH(1)/8 = 0 or 1.

Col. 1-10 11-20 etc.	HVTM(1,J):	Value of concentration (or solute flux if IBTND1 = 0) corresponding to TMHV(1,J), where J = 1,...., NTSNDH(1).

(d) Fluid flux value records (8E10.3)

*** Omit if performing a water flow simulation (IMODL = 1).

Number of records = NTSNDF(1)/8 + 0 or 1.

Col. 1-10 11-20 etc.	QVTM(1,J):	Volumetric water flux values corresponding to TMHV (1,J), where J = 1,...., NTSNDH(1).

Group 14. Time-dependent boundary condition records for node NP

*** Omit if ITCNDN = 0, or if SAFTMOD is on.

If performing a water flow simulation, supply the following information:

(a) Control record (I5)

One record.

Col. 1-5	NTSHDH(2):	Number of selected time values on the time graph of pressure head (or water flux if IBTNDN = 0) at node NP.

(b) Time value records (8E10.3)

Number of cards = NTSNDH(2)/8 + 0 or 1.

Col. 1-10 11-20 etc.	TMHV(2,J):	Time values at the selected interpolation points on the time graph of pressure head (or water flux if IBTNDN = 0) at node NP, where J = 1,...., NTSNDH(2).

(c) Functional value record (8E10.3)

Number of records = NTSNDH(2)/8 + 0 or 1.

Col. 1-10 11-20 etc.	HVTM(2,J):	Value of pressure head (or water flux if IBTNDN = 0) corresponding to TMHV(2,J), where J = 1,...., NTSNDH(2).

If performing solute transport simulation, supply the following information:

(a) Control record (I5)

One record.

Col. 1-5	NTSNDH(2):	Number of selected time values on the time graph of concentration (or solute flux if IBTNDN = 0).

(b) Time value records (8E10.3)

Number of records = NTSNDH(2)/8 + 0 or 1.

Col. 1-10	TMVH(2,J):	Time values at the selected interpolation points on the time graph of concentration (or solute flux if IBTNDN = 0) at node NP, where J = 1,...., NTSNDH(2).
11-20		
etc.		

(c) Functional value record (8E10.3)

Number of records = NTSNDH(2)/8 + 0 or 1.

Col. 1-10	HVTM(2,J):	Value of concentration (or water flux if IBTNDN = 0) corresponding to TMHV(2,J), where J = 1,....,NTSNDH(2).
11-20		
etc.		

(d) Fluid flux value records (8E10.2)

*** Omit if performing a water flow simulation (IMODL = 1).

Number of records = NTSNDH(2)/8 + 0 or 1.

Col. 1-10	QVTM(2,J):	Volumetric water flux values corresponding to TMHV(2,J), where J = 1,..., NTSNDH(2).
11-20		
etc.		

Group 15. Observation node records (16I5)

*** Omit if IOBSND or NOBSND = 0.

Number of records = NOBSND/16 + 0 or 1.

Col. 1-5	NDOBS(I):	Increasing sequential numbers of observation nodes 1 through NOBSND, where J = 1,...., NOBSND.
6-10		
etc.		

4.2.4 SAFTMOD Input

The code is designed to perform the analysis of one flow and/or a flow and associated transport problem when run in the linked mode. An option is provided for automatic generation of default initial values. This option is invoked by setting the input variables NONU and NPIN equal to zero. When this is the case, all nodal values of the dependent variables will be set equal to the default initial values. In addition, the code is designed to allow any set of consistent units to be assigned to the input variables. When run in linked mode, the unit of length is meters. Note that this is different from the length unit used in PRZM and VADOFT, which is centimeters.

The input data required for fluid flow and solute transport simulations are classified into 24 groups given in their sequential order as follows:

1. Problem title
2. Problem control record
3. Simulation control parameter
4. Time stepping and iteration control record
5. Input/output control record
6. Temporal discretization data
7. Mesh generation control data
8. Aquifer identification data
9. Aquifer material property data
10. Aquifer thickness and base elevation data
11. Aquitard identification data
12. Aquitard material property and head data
13. Solute property data
14. Groundwater recharge and pesticide loading data
15. Boundary condition control
16. Steady-state Dirichlet boundary condition data
17. Steady-state flux boundary condition data
18. Transient Dirichlet boundary condition data
19. Transient flux boundary condition data
20. Initial condition data
21. Velocity and saturated thickness data
22. Sequential numbers of nonzero flux nodes
23. Output printout control data
24. Sequential numbers of observation nodes

This sequence must be strictly adhered to when entering the data into the program. If a transport simulation is to follow a flow simulation, the data set defining the transport simulation must immediately follow the data set defining the flow simulation. A sample input file is shown in Figures 6.4 and 6.6. A description of input variables and data formats is presented on the following pages.

Group 1. Title record (A80)

One record.

Col. 1-80 TITLE: Title of problem.

Group 2. Problem control record (8I5)

One record.

Col. 1-5 IMODL: Parameter indicating the type of modeling problem;
= 0 for solute transport modeling,
= 1 for groundwater flow modeling.

6-10	IAREAL:	Parameter indicating orientation of the finite element grid; = 0 if cross-sectional, = 1 if areal. In an cross-sectional analysis, the code assumes that the y-axis is oriented vertically.
11-15	IAXSYM:	Parameter indicating if the cross-sectional analysis is to be performed using axisymmetric coordinates; = 0 if no, = 1 if yes. Note that IAXSYM is automatically set equal to zero if IAREAL = 1.
16-20	NAQFR:	For the case of areal analysis (IAREAL = 1), NAQFR denotes the number of aquifer units, and its value may be equal to 1 or 2. For the case of cross-sectional or axisymmetric analysis (IAREAL = 0), set NAQFR = 1. In any case, NAQFR must be greater than 0 and not greater than 2.
21-25	NAQTRD:	For the case of areal analysis, NAQTRD is a parameter indicating if there is a confining semipermeable layer (aquitard) separating two aquifers; = 0 if no, = 1 if yes. For the case of cross-sectional or axisymmetric analysis, set NAQTRD = 0.
26-30	IWATP:	Parameter indicating the hydraulic boundary condition of the aquifer system; = 0 for confined system, = 1 for unconfined or partially unconfined system.
31-35	IVRECH:	Parameter indicating if precipitation recharge (or infiltration) and water table conditions are to be taken into account in solving the flow or transport problem; = 0 if no, = 1 if yes.
36-40	NZONRT:	Number of zones with time-dependent recharge rates. Set NZONRT = 0 if there are no such zones.

Group 3. Simulation control parameter (8I5)

One record.

Col. 1-5	IEXEC:	Code execution control parameter; = 0 if execution is to be stopped after generation and output of mesh data, = 1 if execution is to continue until simulation is completed.
6-10	ITRANS:	Parameter indicating if the simulation is to be performed in a transient or steady-state mode; = 0 for steady-state simulation, = 1 for transient simulation.
11-15	NTS:	Number of simulation time steps. For a steady-state simulation, NTS is automatically set = 1. In linked mode, this value will be overridden by the value specified in the execution supervisor file.
16-20	ITSGN:	Parameter indicating if simulation time values are to be generated by the code; = 0 if no, = 1 if yes. For a steady-state simulation, ITSGN is automatically set = 1.
21-25	NP:	Total number of nodal points in the finite element grid to be used in the analysis.
26-30	NE:	Total number of elements in the grid.
31-35	IOUTLT:	Parameter indicating if integrated values of fluid or solute fluxes at certain specified nodes are to be determined by the code; = 0 if no, = 1 if yes.
36-40	IMBAL:	Parameter indicating if mass balance computation is required; = 1 if yes, = 0 if no. When IMBAL = 1, IOUTLT should also be equal to 1. Otherwise the code will set IMBAL to zero.

Group 4. Time stepping and iteration control record (2I5, 2E10.3)

One record.

Col. 1-5	IKALL:	Parameter indicating the type of time-stepping scheme required;

		= 0 for central difference, = 1 for backward difference. For a steady-state analysis, IKALL is automatically set = 1.
6-10	NITMAX:	Maximum number of nonlinear iterative solutions allowed per time step. In the case of unconfined or partially unconfined flow, NITMAX should be greater than 1 (recommended value is 5 for transient analysis, and 10 for steady-state analysis). Otherwise, NITMAX should be set equal to 1.
11-15	HTOL:	Iteration tolerance for hydraulic head (or concentration). The selected value of HTOL should be less than or equal to 0.01 of the maximum expected value of head (or concentration). In any case, HTOL must be greater than zero.

Group 5. Input/output control record (11I5)

One record.

Col. 1-5	IPRD:	Parameter indicating printed output requirements pertaining to the finite element mesh and initial condition data; = 0 if mesh and initial condition data are to be printed, = 1 if element identification data printout is not required, = 2 if the entire mesh data printout is not required, = 3 if mesh and initial condition data printouts and boundary condition print checks are not required.
6-10	NSTEP:	Parameters controlling the interval of printing of computed values of head (or concentration) at all nodal points. When NSTEP = n, these nodal values are printed for each nth time step. If the nodal printout is to be suppressed for all time steps, set NSTEP = 0.
11-15	NVPR:	Parameter controlling printout of element Darcy velocities. When NVPR = n, these velocities are printed for each nth time step. If the velocity printout is to be suppressed for all time steps, set NVPR = 0.

16-20 NOWRIT: Parameter indicating if computed values of head (or concentration) at the final time level are to be written to a scratch file;
= 0 if no,
= 1 if yes.
Note: The purpose of the NOWRIT = 1 option is to create head or concentration data that can be used as the initial condition for a restart run.

21-25 NVWRIT: Parameter specifying if computed element velocities and, if needed, nodal values of saturated thickness are to be written to a scratch file for use in the associated transport run;
= 0 if no output is to be written,
= 1 if the output is to be written.
NVWRIT is irrelevant in the transport simulation and is automatically set = 0.

26-30 NPLOT: Parameter specifying if time and computed values of head or concentration are to be written for use in subsequent plotting;
= 0 if no output is to be written,
= n if the output is to be written for each nth time step.

31-35 NVREAD: Parameter specifying if element Darcy velocity and saturated thickness data are to be input using a separate scratch data file;
= 0 if no,
= 1 if yes.
In the flow simulation (IMODL=1), the code automatically sets the value of NVREAD equal to 0 to avoid reading a velocity file.

36-40 IVSTED: Parameter indicating if the velocity field to be used in the transport simulation is in steady-state;
= 0 if no,
= 1 if yes.

41-45 IOBSND: Parameter indicating if values at some specified nodes are to be recorded and printed for all time steps;
= 0 if no,
= 1 if yes.

46-50 IPRCON: Parameter indicating if the output printout windowing option is to be used;
= 0 if no,
= 1 if yes.

51-55 IPRCHK: Matrix computation print check parameter;
= 0 if print checks are not needed,
= 1 if print checks are needed.
(This parameter controls the printing of intermediate matrix calculations. It should normally be set to zero, but for it to be effective the echo level defined in the Execution Supervisor input should be set to 6 or greater.)

Group 6. Temporal discretization data

*** Omit if PRZM is on or if VADOFT is on.

(a) Time step control parameters (4E10.3)

*** Omit if ITRANS (group 3, parameter 2) = 0, or if ITSGN (group 3, parameter 4) = 0.

One record.

Col. 1-10 TIMA: Starting time value of the simulation.

11-20 TIN: Value of the first time step.

21-30 TFAC: Multiplier used to compute values of subsequent time steps.

31-40 TMAX: Maximum allowable value of time step generated by the code.

(b) User-supplied time values (8E10.3)

*** Omit if ITRANS = 0, or if ITSGN = 1.

Number of records = NTS/8 + (0 or 1).

Col. 1-10 TMVEC(I): Time values at the end of time
11-20 steps 1 through NTS, where I = 1,...., NTS.
etc.

Group 7. Mesh generation control data

These data are required by the code to generate a rectangular finite element mesh. Nodal coordinates are set up along the x and y axes. In the case of areal simulation, these axes lie in an areal flow plane. In the case of vertical cross-sectional simulation, x and y axes are oriented in the horizontal and vertical directions, respectively. In the case of axisymmetric simulation, the x and y coordinates correspond to the radial and vertical cylindrical coordinates, respectively.

(a) Control parameter record (5I5)

One record.

Col. 1-5	NROWS:	Number of nodal grid lines parallel to the direction of the x-axis. NROWS must be greater than or equal to 2.
6-10	NCOLS:	Number of nodal grid lines parallel to the direction of the y-axis. NCOLS must be greater than or equal to 2.
11-15	IXYRED:	Parameter indicating if coordinates of the grid lines parallel to x and y axes are to be input; = 0 if no, = 1 if yes.
16-20	ISWAP:	Parameter indicating the sequential numbering of the nodes in the rectangular mesh to be generated; = 0 if the nodes are sequentially numbered in the y-direction, = 1 if the nodes are sequentially numbered in the x-direction. The purpose of ISWAP is to achieve a smaller matrix bandwidth.
21-25	ICOVR:	Parameter indicating if nodal coordinates generated by the code are to be overridden by user-supplied values; = 0 if no, = 1 if yes.

(b) Mesh spacing control parameters (8E10.3)

*** Omit if IXYRED = 1.

One record.

Col. 1-10	DX:	Nodal spacing in the x-direction of the first grid block.
11-20	DY:	Nodal spacing in the y-direction of the first grid block.
21-30	SCFX:	Multiplier used to compute values of remaining nodal spacings in the x-direction.
31-40	SCFY:	Multiplier used to compute values of remaining nodal spacings in the y-direction.

41-50 DXMAX: Maximum allowable value of nodal spacing in the x-direction.

51-60 DYMAX: Maximum allowable value of nodal spacing in the y-direction.

61-70 XO: Length along the x-direction of the discretized rectangular region.

71-80 YO: Length along the y-direction of the discretized rectangular region.

(c) User-supplied x-coordinates of grid lines (8E10.3)

*** Omit if IXYRED = 0.

Number of records = NCOLS/8 + (0 or 1).

Col. 1-10 XW(J): x-coordinates of grid lines 1 through
11-20 NCOLS, WHERE J = 1,...., NCOLS.
etc.

(d) User-supplied y-coordinates of grid lines (8E10.3)

*** Omit if IXYRED = 0.

Number of records = NROWS/8 + (0 or 1).

Col. 1-10 YW(J): y-coordinates of grid lines 1 through
11-20 NROWS, where J = 1,...., NROWS.
etc.

(e) User-supplied nodal coordinates (I5, 2E10.3)

*** Omit if ICOVR = 0.

Number of records = NP.

Col. 1-5 N: Node number.
6-15 CORD (N,1): x-coordinate.
16-20 CORD (N,2): y-coordinate.

Group 8. Aquifer identification data

(a) General identification records (3I5)

Number of records = NAQFR.

Each record contains the following information:

Col. 1-5 I: Aquifer unit number.
6-10 NMATAQ(I): Number of different soil materials in aquifer unit I. In determining the value of NMATAQ(I), disregard the zones where the material number is assigned zero value.
11-15 IAQTYP(I): Type of aquifer unit I;
= 0 for confined aquifer,
= 1 for unconfined or partially unconfined aquifer.

(b) Aquifer material identification records (6I5)

Number of records = as many as needed.

Each record contains the following information:

Col. 1-5 IAQFR: Aquifer unit number.
6-10 IZONO: Material number assigned to a particular zone of the aquifer. Ignore zones that are impermeable or outside the modeled region. For those zones the code automatically sets IZONO = 0.
11-15 IEST: Starting sequential element number in the specified material zone.
16-20 IEFIN: Ending sequential element number in the specified material zone.
21-25 IEINCR: Element number increment.
26-30 IPAUSE: Parameter indicating if this record is the last record in this group;
= 0 if no,
= 1 if yes.

Group 9. Aquifer material property data (5E10.3)

There is one set of records per aquifer unit. Record set L contains properties of soil materials in aquifer unit L.

For IMODL = 1 (flow modeling), each record contains the following information pertaining to porous material number I in aquifer L:

Number of records in the set = NMATAQ(L).

Col. 1-10 PROP(I,L,1): Hydraulic conductivity component K_{xx} of material number I in aquifer unit L.
11-20 PROP(I,L,2): Hydraulic conductivity component K_{yy} of material number I in aquifer unit L.
21-30 PROP(I,L,3): Specific storage of material I in aquifer unit L. (Enter 0 if flow is steady-state).
31-40 PROP(I,L,4): Specific yield of material I in aquifer unit L. (Enter 0 if flow is steady-state and/or the aquifer is confined).

41-50	PROP(I,L,5):	Hydraulic conductivity component K_{zz} of material number I in aquifer unit L. In the areal flow simulation, K_{zz} corresponds to the vertical hydraulic conductivity, and is not allowed to exceed 0.1*minimum (K_{xx}, K_{yy}). In the cross-sectional or axisymmetric flow simulation, the code automatically sets $K_{zz}=K_{yy}$.

For IMODL = 0 (transport modeling), each record or group of records contains the following information pertaining to porous material number I in aquifer L:

Number of records = (1 + (NCHEM-1))NMATAQ(L)

(a)	Col. 1-10	PROP(I,L,1):	Longitudinal dispersivity of material I in aquifer unit L.
	11-20	PROP(I,L,2):	Transverse dispersivity of material I in aquifer unit L.
	21-30	PROP(I,L,3):	Molecular diffusion coefficient component D_o of material I in aquifer unit L for first chemical.
	31-40	PROP(I,L,4):	Effective porosity of material I in aquifer unit L.
	41-50	PROP(I,L,5):	Vertical dispersivity of material I in aquifer unit L. Note that in the cross-sectional or axisymmetric simulation, the code automatically sets PROP (I,L,5) = PROP (I,L,2).

(b) Molecular diffusion coefficient component D_o of material I in aquifer unit L for remaining chemicals (20X, F10.0)

*** Omit if NCHEM (defined in RUSTIC.RUN) is less than 2.

Number of records = NCHEM - 1.

Col. 21-30	CPROP (I,L,ICHEM):	Molecular diffusion coefficient component D_o of material I in aquifer unit L of chemical ICHEM.

Group 10. Aquifer thickness and base elevation data (I5, 2E10.3, 4I5)

*** Omit if performing transport analysis (IMODL=0) or performing cross-sectional or axisymmetric flow analysis (IAREAL=0).

Number of records = as many as needed. Each record contains the following information:

Col. 1-5	IAQFR:	Aquifer unit number.
6-15	ZBASE:	Zonal value of elevation of the aquifer base above the datum plane.
16-25	THCKMX:	Zonal value of total thickness of the aquifer unit. If THCKMX is not specified, the code assumes an infinite thickness.
26-30	INDST:	Starting sequential node number in this zone.
31-35	INDEND:	Ending sequential node number in this zone.
36-40	NDINCR:	Nodal increment.
41-45	IPAUSE:	Parameter indicating whether this record is the last record in this group; = 0 if no, = 1 if yes.

Group 11. Aquitard identification data

*** Omit if there is no aquitard (NAQTRD = 0).

(a) General identification data (3I5)

One record.

Col. 1-5	NMATRD:	Number of different soil materials in the aquitard unit.
6-10	NPATCO:	Number of nodal points in each aquitard column. For a steady-state simulation, NPATCO is automatically set equal to 2. For a transient simulation, suggested value of NPATCO is between 5 and 10.
11-15	IZATRD:	Parameter indicating if the dimensionless vertical coordinate of the aquitard is to be read; = 0 if no, = 1 if yes.

(b) Aquitard material identification records (5I5)

Number of records = as many as needed. Each record contains the following information:

Col. 1-5	IZONO:	Material number assigned to a particular zone of the aquitard.
6-10	ICOLST:	Starting sequential number of the vertical aquitard-soil column in the zone.
11-15	ICOLEN:	Ending sequential number of the vertical aquitard-soil column in the zone.
16-20	ICINCR:	Increment of sequential column numbers.
21-25	IPAUSE:	Parameter indicating whether this record is the last record in this group; = 0 if no, = 1 if yes.

(c) Dimensionless vertical coordinates of aquitard (8E10.3)

*** Omit if IZATRD = 0.

Number of records = NPATCO/8 + 0 or 1.

Col. 1-10 11-20	DIST(I):	Nodal values of dimensionless transverse coordinate in the aquitard layer where I = etc.1,...., NPATCO.

Group 12. Aquitard material property and head data (3E10.3)

*** Omit if there is no aquitard (NAQTRD=0).

Number of records = NMATRD.

For IMODL = 1 (flow modeling), each record contains the following information pertaining to porous material number I of the aquitard:

Col. 1-10	ATPROP(I,1):	Vertical component of saturated hydraulic conductivity of material I in the aquitard.
11-20	ATPROP(I,2):	Specific storage of material I in the aquitard.
21-30	ATPROP(I,3):	Thickness of material I in the aquitard.

For IMODL = 0 (transport modeling), each record contains the following information pertaining to material number I of the aquitard:

Col. 1-10	ATPROP(I,1):	Dispersion coefficient for material I in the aquitard.
11-20	ATPROP(I,2):	Porosity of material I in the aquitard.
21-30	ATPROP(I,3):	Thickness of aquitard material I in the aquitard.

Group 13. Solute property data and default overriding values

*** Omit if performing groundwater flow analysis (IMODL=1).

(a) Aquitard default solute property values (2E10.3)

*** Omit if NAQTRD (group 2, parameter 5) = 0.

One record.

Col. 1-10	RPCOEF:	Default value of retardation coefficient assigned to the aquitard.
11-20	DPLAM:	Default value of decay coefficient assigned to the aquitard.

(b) Default overriding control parameters (2I5)

One record.

Col. 1-5 IATROR: Parameter indicating if assigned aquitard default values are to be overridden;
= 0 if no,
= 1 if yes.

(c) Aquitard overriding solute property values (2E10.3,4I5)

*** Omit if IATROR = 0.

Number of records = as many as needed. Each record contains the following information:

Col. 1-10 RPCOR: Overriding value of retardation coefficient in the aquitard.
11-20 DPLOR: Overriding value of decay coefficient.
21-25 ICOLST: Starting sequential number of aquitard column having the overriding solute property values.
26-30 ICINCR: Ending sequential number of aquitard column having the overriding solute property values.
31-35 ICINCR: Increment of column numbering in the aquitard zone having the overriding solute property values.
36-40 IPAUSE: Parameter indicating if this record is the last record in subgroup 13(c).

(d) Transport parameter records (3E10.3)

Number of records = NAQFR * NMATAQ (IAQ) * NCHEM. (Values should be defined for all chemicals in material 1 of aquifer 1, then all chemicals in material 2 of aquifer 1, etc.)

Col. 1-10 RCOFP(IMAT,IAQ,ICHEM): Aquifer retardation coefficient in material IMAT of aquifer IAQ, for chemical ICHEM
11-20 DLAMP(IMAT,IAQ,ICHEM): Decay coefficient of chemical ICHEM in material IMAT of aquifer IAQ
21-30 FRACMP(IMAT,IAQ,ICHEM): Transformation of chemical ICHEM in material IMAT of aquifer IAQ.

Group 14. Groundwater recharge and solute (pesticide) loading data

*** Omit groups 14a-14b if IVRECH (record group 2, col, 31-35) is equal to zero.

(a) Groundwater recharge control records (I5, E10.3, 4I5)

Number of records = as many as needed. Each record contains the following information:

In preparing the data in this group, special attention should be paid to the case of cross-sectional or axisymmetric analysis involving an unconfined aquifer system. For this case, all top boundary nodes of the grid that need to receive specific yield treatment must be identified and included in this data group. Hence, for this case, the zone with zero recharge value must also be included. For other cases, the zone(s) with zero recharge value may be omitted.

Col. 1-5	IRZON:	Recharge zone number.
6-15	RCHVAL:	Steady-state default value of the recharge rate for the zone. A dummy value for RCHVAL may be set if NZONRT is greater than zero (see next card group) or PRZM or VADOFT is on. In either of these cases, RCHVAL will not be used.
16-20	INDMIN:	Lowest sequential nodal number in the recharge zone.
21-25	INDMAX:	Highest sequential nodal number in the recharge zone.
26-30	NDINCR:	Nodal increment.
31-35	IPAUSE:	Parameter indicating if this is the last record in this group: = 0 if no, = 1 if yes.

(b) Transient recharge records

*** Omit if NZONRT (record group 2, col. 36-40) is equal to zero.

Number of record sets = NZONRT.

These records are divided into three subgroups as follows:

(i) Control record (2I5)

One record.

Col. 1-5	IRZON:	Recharge zone number.
6-10	NTSRCH:	Number of control (interpolation) points on the graph of recharge rate versus time. Set to 2 when running with VADOFT or PRZM on.

(ii) Time value records (8E10.3)

Number of records = NTSRCH

Col. 1-10
11-20
21-30
etc.

TMRCH(IRZON,J): Time values corresponding to control points on the graph of recharge rate versus time, where J = 1,...., NTSRCH. (When running with PRZM or VADOFT ON, dummy values may be entered as they will be overridden during the simulation).

(iii) Recharge value records (8E10.3)

Number of records = NTSRCH.

Col. 1-10
11-20
21-30
etc.

RCHTM(IRZON,J): Recharge rate values corresponding to control points on the graph of recharge rate versus time. Dummy values may be entered if either PRZM or VADOFT is ON as they will be overridden during the simulation by fluxes from either of the two models, where J = 1,...., NTSRCH.

(c) Solute (pesticide) loading zone identification records

These records are divided into two subgroups as follows:

(i) Control record (2I5)

One record.

Col. 1-5 IPSZP: Zone number (must be 1 in current version of RUSTIC).

6-10 NDCOUN: Number of nodes in the zone.

(ii) Zone identification records (16I5)

Col. 1-5
6-10
etc.

NDIDEN(I,IPSZO): Node numbers of the nodes that lie in zone #IPSZO, where I = 1,...., NDCOUN.

(d) Solute (pesticide) mass loading records

These records are divided into three subgroups as follows:

(i) Control record (2I5)

Col. 1-5 IPSZO: Zone number (must be 1 in current version of RUSTIC).

6-10 NTSPSZ: Number of control (interpolation) points on the graph of solute mass application rate versus time.

(ii) Time value records (8E10.3)

Number of records = NTSPSZ.

Col. 1-10 11-20 21-30 etc.	TMPSZ(IPSZO,J):	Time values corresponding to control points on the graph of solute mass application rate versus time, where J=1,....., NTSPSZ. When running with PRZM or VADOFT ON, dummy values may be entered as they will be overridden during the simulation.

(iii) Solute mass application rate records (8E10.3)

Number of records = NTSPSZ.

Col. 1-10 11-20 21-30 etc.	SFLXTM(IPSZO,J):	Values of solute mass application rate corresponding to control points on the graph of solute mass application rate versus time, where J=1,....,NTSPSZ. Dummy values may be entered if either PRZM or VADOFT is ON as they will be overridden during the simulation by fluxes from either of the two models.

Group 15. Boundary condition control record (4I5)

One record.

Col. 1-5	NBTO:	Number of nodes where steady-state functional values (hydraulic head or concentration) are prescribed.
6-10	NDFLUX:	Number of nodes where steady-state fluid (or solute) flux values are prescribed.
11-15	NBHVAR:	Number of boundary nodes for which functional values (hydraulic head or concentration) are time dependent.
16-20	NBFVAR:	Number of boundary nodes for which fluid (or solute) flux values are time dependent.

Note: In determining the values of NDFLUX and NBFVAR, do not count those groundwater recharge or pesticide flux nodes if they have already been accounted for in record group 14.

Group 16. Steady-state Dirichlet boundary condition data (I5,E10.3)

*** Omit if NBTO = 0.

Number of records = NBTO. Each record contains the following information:

Col. 1-5 NODV(I): Aquifer node number.
6-15 VAVO(I): Prescribed value of the unknown function (head or concentration).

Group 17. Steady-state flux boundary condition data (I5,2E10.3)

*** Omit if NDFLUX = 0.

Number of records = NDFLUX. Each record contains the following information:

Col. 1-5 NODF(I): Aquifer node number.
6-15 FLUXVO(I): For groundwater flow analysis (IMODL=1), FLUXVO(I) denotes the net integrated fluid flux ($L^1 T^{-1}$) at the aquifer node. For solute transport analysis (IMODL=0), FLUXVO(I) denotes the net solute flux (MT^{-1}) entering the aquifer node.

16-25 QVALV(I): For groundwater flow analysis (IMODL=1), set QVALV(I) = 0 or leave blank. For solute transport analysis, QVALV(I) denotes the net volumetric fluid flux entering the aquifer node.

Note: The sign convention for fluxes is positive for influxes and negative for effluxes. In performing solute transport simulation, the code automatically treats the nodes that correspond to pumping wells and efflux boundary nodes. Hence, such nodes can be excluded from data group 17.

Group 18. Transient Dirichlet boundary condition data

*** Omit if NBHVAR = 0.

Number of record sets = NBHVAR.

Each set contains the following records:

(a) Control record (3I5)

One record.

Col. 1-5 NDHVAR(I): Node number of a time-dependent Dirichlet (prescribed head or concentration) node in the aquifer region.
6-10 NTSNDH(I): Number of control (interpolation) points on the graph of the function (head or concentration) versus time.

11-15	IREPB:	Parameter indicating if transient boundary condition data in record types 18b and 18c of this record set are the same as those of the preceding record set; = 1 if yes, = 0 if no.

(b) Time value records (8E10.3)

*** Omit if IREPB = 1.

Number of records = NTSNDH(I)/8 + (0 or 1).

Col. 1-10 11-20 etc.	TMHV(I,J):	Time values corresponding to control points on the graph of function (head or concentration) versus time, where J = 1,....,NTSNDH(I).

(c) Functional value records (8E10.3)

*** Omit if IREPB = 1.

Number of records = NTSHDN(I)/8 + (0 or 1).

Col. 1-10 11-20 etc.	HVTM(K,J):	Value of function (head or concentration) corresponding to TMHV(I,J), where J = 1,...., NTSNDH(I).

Group 19. Transient flux boundary condition data

*** Omit if NBFVAR = 0.

Number of record sets = NBFVAR. Each set contains the following information:

(a) Control record (3I5)

One record.

Col. 1-5	NDFVAR(I):	Node number of a time-dependent flux boundary node in the aquifer region.
6-10	NTSNDF(I):	Number of control (interpolation) points on the graph of fluid (or solute) flux versus time.
11-15	IREPB:	Parameter indicating if transient boundary condition data in record types 19b-19d are the same as those of the preceding record set; = 0 if no, = 1 if yes.

(b) Time value records (8E10.3)

*** Omit if IREPB = 1.

Number of records = NTSNDF(I)/8 + (0 or 1).

Col. 1-10 11-20 etc.	TMHF(I,J):	Time values corresponding to control points on the graph of fluid (or solute flux versus time, where J = 1, ..., NTSNDF(I).

(c) Flux value records (8E10.3)

*** Omit if IREPB = 1.

Number of records = NTSNDF(I)/8 + (0 or 1).

Col. 1-10 11-20 etc.	FVTM(I,J):	For groundwater flow analysis, interpret these as volumetric fluid flux values corresponding to TMHF (I,J). For solute transport analysis, interpret these as injected mass flux values corresponding to TMHF (I,J), where J = 1, ..., NTSNDF(I).

(d) Fluid flux value records (8E10.3)

*** Omit if performing groundwater flow analysis (IMODL=1) or if IRPEB = 1.

Number of records = NTSNDF(I)/8 + (0 or 1).

Col. 1-10 11-20 etc.	QVTM(I,J):	For solute transport analysis, interpret these as injected fluid volumetric flux values corresponding to TMHF(I,J), where J = 1,...., NTSNDF(I).

Note: In performing solute transport simulation, the code automatically treats the nodes that correspond to pumping wells and efflux boundary nodes. Hence, such nodes can be excluded from data group 19.

Group 20. Initial condition data

(a) Default initial values for aquifers (2E10.3)

One record.

Col. 1-10 11-20	HIAQFR(I):	Default initial values of hydraulic head (or concentration) in aquifer unit 1 to NAQFR, where I = 1, 2.

(b) Default initial value for aquitard (E10.3)

*** Omit if there is no aquitard (NAQTRD = 0).

One record.

Col. 1-10	HIATRD:	Default initial value of hydraulic head (or concentration) in the aquitard.

(c) Initial condition control parameters (3I5)

One record.

Col. 1-5	NONU:	Parameter indicating the uniformity of the initial condition; = 0 if the initial condition is uniform and may be expressed using the default values, = 1 if the initial condition is nonuniform and may be described using the default initial values in conjunction with the overriding initial value input option (subgroup 20 (d)), = 2 if the initial condition is nonuniform and the initial values are to be supplied from a separate data file, unit number 8. The value of NONU = 2 is normally used when performing a restart simulation.
6-10	NPIN:	Number of nodes where overriding initial values need to be input and included in this data file. The value of NPIN must be set to zero when NONU = 0 or NONU = 2.
11-15	NPINAT:	Number of aquitard columns where overriding initial values need to be input and included in this data file. The value of NPINAT must be set to zero when NONU = 0 or NONU = 2.

(d) Overriding initial values for aquifer nodes (5(I5,E10.3))

*** Omit if NPIN = 0.

Number of records = NPIN/5 + 0 or 1.

Col. 1-5	NDNO:	Node number.
6-10 etc.	HINT(NDNO):	Overriding initial value of hydraulic head (or concentration), where NDNO = 1,...., NPIN.

(e) Overriding initial values for aquitard columns (5(I5,E10.3))

*** Omit if NPINAT = 0.

Number of records = NPINAT/5 + 0 or 1.

Col. 1-5	ICOL:	Column number.
6-10 etc.	HICOL(ICOL):	Overriding initial value of hydraulic head (or concentration), where ICOL = 1,...., NPINAT.

Group 21. Velocity and saturated thickness data (I5,3E10.3,2I5)

*** Omit if performing flow simulation (IMODL=1).

(a) Default velocity and saturated thickness values

Number of records = NAQFR.

Col. 1-5	IAQFR:	Aquifer unit number.
6-15	VXDF:	Default value of Darcy velocity component in the x-direction.
16-25	VYDF:	Default value of Darcy velocity component in the y-direction.
26-35	STHDF:	Default value of aquifer saturated thickness. Note: For a cross-sectional or axisymmetric simulation, the code automatically sets STHDF = 1.
36-40	NEOVEL:	Number of elements that need overriding velocity values.
41-45	NEOTHK:	Number of elements that need overriding saturated thickness values.

(b) Overriding Darcy velocity values (2(I5,2E10.3))

*** Omit if NEOVEL = 0.

Number of records = NEOVEL/2 + 0 or 1.

Col. 1-5	IEL:	Element number.
6-15	VELX(IEL):	Overriding value of x-velocity component.
16-30 etc.	VELY(IEL):	Overriding value of y-velocity component IEL = 1,...., NOEVEL.

(c) Overriding saturated thickness values (5(I5,E10.3))

*** Omit if NEOTHK = 0.

Number of records = NEOTHK/5 + 0 or 1.

Col. 1-5	IEL:	Element number.
6-15 etc.	THEL(IEL):	Overriding value of saturated thickness, where IEL = 1,...., NEOTHK.

Group 22. Sequential numbers of nonzero flux nodes

*** Omit if IOUTLT (group 3, parameter 7) = 0.

(a) Control parameter (I5)

One record.

Col. 1-5	NBOUT:	Number of aquifer nodes where the net integrated fluid or solute flux values are nonzero.

(b) Sequential node numbers (16I5)

Number of records = NBOUT/16 + (0 or 1).

Col. 1-5 6-10 etc.	NDOUT(I):	Sequential numbers of the nodes where the flux values are required, where I = 1,...., NBOUT.

(c) Computed values of fluid fluxes (8E10.3)

*** Omit if performing fluid flow simulation (IMODL=1) or if performing transport simulation (IMODL=0) but using the option (NVREAD=1) by which velocity and fluid flux data are supplied to the code from file unit 9.

Number of records = NBOUT/8 + 0 or 1.

Col. 1-10 11-20 etc.	QNDOUT(I):	Net values of volumetric fluid fluxes at the nodes, where I = 1,...., NBOUT.

Group 23. Output printout control data

*** Omit if IPRCON (group 5, parameter 10) = 0.

(a) Control parameters (2I5)

One record.

Col. 1-5	NTCLIP:	Number of time values at which head (or concentration) values at selected nodes are to be printed.
6-10	NWINDO:	Number of output window sections in the modeled region.

(b) Selected time values (8E10.3)

Number of records = NTCLIP/8 + (0 or 1).

Col. 1-10 11-20 etc.	TMCLIP(I):	Time values at which head (or concentration) values in the window sections are to be printed. These time values must be arranged in order of increasing magnitude, where I = 1, ..., NTCLIP.

(c) Windowing section data (9I5)

Number of records = as many as needed.

Col. 1-5	IWNO:	Window section number.
6-10	INDST:	Starting aquifer node number of output traversing line (transect).
11-15	INDEND:	Ending aquifer node number of output transect.
16-20	NDINCR:	Nodal increment.

*** If printed output for aquitard columns are not required, leave columns 21-35 blank.

21-25	ICOLST:	Starting sequential number of aquitard column passing through output transect.
26-30	ICOLEN:	Ending sequential number of aquitard column passing output transect.
31-35	ICINCR:	Column number increment.
36-40	IRECW:	Parameter indicating if this record is the first record for window number IWNO; = 0 if no, = 1 if yes.
41-45	IPAUSE:	Parameter indicating if this record is the last record of subgroup 23(c); = 0 if no, = 1 if yes.

Group 24. Sequential numbers of observation nodes

*** Omit if IOBSND (group 5, parameter 9) = 0.

(a) Control record (I5)

One record.

Col. 1-5	NNOBS:	Number of observation nodes for which continuous monitoring of head (or concentration) versus time is required.

(b) Sequential node numbers (16I5)

Number of records = NNOBS/16 + (0 or 1).

Col. 1-5 6-10 etc.	NDOBS(I):	Sequential numbers of observation nodes, where I = 1,...., NNOBS.

4.2.5 The Monte Carlo Input

The Monte Carlo module uses one input file to specify the distributions of variables and to select output options. This section describes the format of this input file and the available user options. A sample input file is shown in Figure 4.5.

The Monte Carlo input file consists of data lines and two types of general utility lines. The first type of utility line is the comment line, indicated by the presence of three asterisks ('***') as the first non-blank characters in the line. These lines are ignored by the model and are provided to allow the user to type in comments, table headings, and other information useful in making the input file more understandable. Comment lines may be inserted anywhere in the data set. The second type of utility line is the END line, used by the code to mark the end of specific data groups. These lines are indicated by the word 'END' in the first three columns of the input line, and should be used only where specified in the following discussion.

Monte Carlo input data are comprised of five data groups: (1) simulation control parameters, (2) input distribution parameters, (3) empirical distribution data, (4) output options, and (5) correlated variable input. Data are read sequentially starting with Data Group 1 and ending with Data Group 5. Specific formats for each Data Group are shown below.

4.2.5.1 Data Group 1: Simulation Control Parameters--

This data group consists of two lines of data describing simulation options. The first line contains the (alphanumeric) title for the run and is used to label the output. The second line contains the number of Monte Carlo runs and the percentile confidence level to be used in the simulation.

RECORD 1. TITLE

FORMAT(A80)

TITLE (80): Title for Monte Carlo simulation.

RECORD 2. NRUNS, PALPH

FORMAT(I5,F10.0)

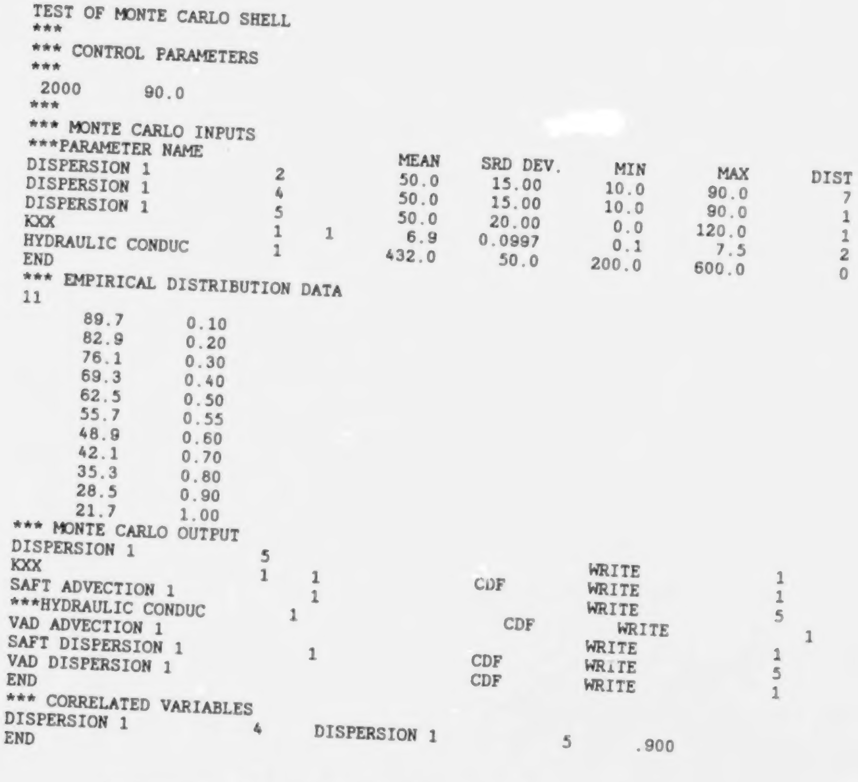
NRUNS: Number of Monte Carlo runs.
PALPH: Confidence level for percentile confidence bounds, entered as a percent (%).

4.2.5.2 Data Group 2: Input Distribution Parameters--
This data group consists of one line of data for each model parameter to be varied (i.e., random input variables). The first entry on each line is a label, of length up to 20 characters, and 2 array indices used to identify the parameter to be varied. The remaining data on these lines consist of frequency distribution parameters for the selected variables. After a data line is provided for each desired random variable, an END card must be supplied to mark the end of this data group. Note that by setting the distribution flag VAR(5) to 0, the user can specify a parameter as a constant. In this case, the mean value of the parameter will be used in the simulations. This option allows the user to vary the parameters to be Monte Carloed without extensive modification of the input file. The user should be aware that parameters which are designated as constants in the Monte Carlo input file are used in lieu of the same parameter value in the standard input file.

<u>RECORD 3</u>. PNAME(20), INDI, INDZ, VAR(1), VAR(2), VAR(3), VAR(4), VAR(5)

FORMAT(A20, 2I5, 5F10.0)

PNAME(20) A label of up to 20 characters identifying the parameter to be varied. Labels used for various parameters are shown in



```
TEST OF MONTE CARLO SHELL
***
*** CONTROL PARAMETERS
***
 2000       90.0
***
*** MONTE CARLO INPUTS
***PARAMETER NAME
DISPERSION 1                           MEAN    SRD DEV.    MIN       MAX       DIST
DISPERSION 1          2                50.0     15.00      10.0      90.0         7
DISPERSION 1          4                50.0     15.00      10.0      90.0         1
KXX                   5                50.0     20.00       0.0     120.0         1
                      1     1           6.9    0.0997       0.1       7.5         2
HYDRAULIC CONDUC      1               432.0      50.0     200.0     600.0         0
END
*** EMPIRICAL DISTRIBUTION DATA
11
      89.7      0.10
      82.9      0.20
      76.1      0.30
      69.3      0.40
      62.5      0.50
      55.7      0.55
      48.9      0.60
      42.1      0.70
      35.3      0.80
      28.5      0.90
      21.7      1.00
*** MONTE CARLO OUTPUT
DISPERSION 1          5
KXX                                                 WRITE              1
                      1    1                 CDF    WRITE              1
SAFT ADVECTION 1           1                        WRITE              5
***HYDRAULIC CONDUC      1                     CDF     WRITE              1
VAD ADVECTION 1                                     WRITE              1
SAFT DISPERSION 1          1                 CDF    WRITE              5
VAD DISPERSION 1                             CDF    WRITE              1
END
*** CORRELATED VARIABLES
DISPERSION 1          4    DISPERSION 1          5     .900
END
```

Figure 4.5. Example MONTE CARLO input file.

Tables 4.7, 4.8 and 4.9. (These tables are located at the end of Section 4.)

INDI: An index for the soil horizon number, application number, or material number corresponding to the parameter identified by PNAME. Appropriate indexes are shown in Tables 4.7, 4.8, and 4.9.

INDZ: For SAFTMOD variables, INDZ refers to the aquifer number corresponding to the variable PNAME. Leave blank for PRZM and VADOFT variables.

VAR(1): The mean of the distribution
VAR(2): The standard deviation of the distribution
VAR(3): The minimum value for the random variable
VAR(4): The maximum value for the random variable
VAR(5): A flag specifying the distribution of the random variable:
0 = Constant
1 = Normal
2 = Log-Normal
3 = Exponential
4 = Uniform
5 = Johnson SU
6 = Johnson SB
7 = Empirical distribution, to be supplied in Data Group 3.
8 = Triangular

4.2.5.3 Data Group 3: Empirical Distribution Data--

This data group contains the piecewise linear descriptions of cumulative frequency distributions for empirically distributed parameters specified in Data Group 2 (by setting the value of VAR(5) to 7). Empirical distributions are read in the order in which parameters were read in Data Group 2. The first data line for each distribution contains the number of data pairs NDAT used to describe the cumulative distribution. This is followed by NDAT data lines, each containing (1) a value of the parameter and (2) the corresponding cumulative probability, expressed as a decimal between 0.0 and 1.0, for the specified value. These data pair lines should be supplied in order of increasing cumulative probability. If no parameters are empirically distributed, then this data group is not necessary.

RECORD 4. NDAT

FORMAT(I5)

NDAT: Number of data pairs used to describe the piecewise linear cumulative distribution.

RECORD 5. DIST(I,1), DIST(I,2)

FORMAT(2F10.0)

DIST(I,1): The value (quantile) for data pair I.
DIST(I,2): The cumulative probability associated with the quantile DIST(I,1).

4.2.5.4 Data Group 4: Output Options--

This data group specifies the statistical output options for each parameter to be written out. This data group consists of one line for each output parameter containing: (1) a character label up to 20 characters long and two array indexes identifying the output parameter, (2) a flag indicating if a cumulative distribution should be plotted for this parameter (selected by supplying the "CDF" here), (3) a flag indicating if values of the parameter are to be written out for each Monte Carlo run (selected by supplying the word "WRITE" here), and (4) the averaging period for output. Labels used to identify input parameters or output variables for PRZM, VADOFT, and SAFTMOD parameters are shown in Tables 4.7, 4.8 and 4.9. A statistical summary table will be printed out for all parameters selected in this data group. An END card is supplied to mark the end of this Data Group after a data line is supplied for each output parameter.

RECORD 6. SNAME(1), INDI, INDZ, SNAME(2), SNAME(3), NAVG

FORMAT(A20, 2I5, 2A20, I5)

SNAME(1):	A label used to identify which parameter is to be statistically summarized.
INDI:	The index for the output parameter (see Tables 4.7, 4.8 and 4.9).
INDZ:	The aquifer number for SAFTMOD output parameters. Leave blank for PRZM and VADOFT parameters.
SNAME(2):	A flag which indicates if cumulative distributions should be plotted for the parameter SNAME(1). This option is selected by inputting "CDF" here.
SNAME(3):	A flag which indicates if values of the parameter are to be written out for each Monte Carlo run (selected by inputting "WRITE" here).
NAVG:	The length of the averaging period for the output parameter. All time series model outputs are written out as maximum N-day moving average values for each Monte Carlo run. Thus, if N=1, statistics are calculated for the maximum daily value. If N=5, statistics are calculated for the maximum 5-day average value in each Monte Carlo run. For PRZM variables, NAVG is the number of days in the average moving period (N). For VADOFT and SAFTMOD variables, NAVG is the number of SAFTMOD time steps in the averaging period.

4.2.5.5 Data Group 5: Correlated Input Variables--

This data group is used to indicate which of the input parameters specified in Data Group 2 are correlated. Note that only parameters with normal, log-normal, Johnson SU, and/or Johnson SB distributions can be correlated. One line of data is provided for each pair of correlated parameters. The first two entries on this line are labels identifying the two parameters that are

TABLE 4-7. MONTE CARLO LABELS FOR PRZM VARIABLES

Parameter	Monte Carlo Label	Index
Random Model Inputs		
Soil Bulk Density (g/cm^3)	BULK DENSITY	Horizon
Wilting Point (cm^3/cm^3)	WILTING POINT	Horizon
Field Capacity (cm^3/cm^3)	FIELD CAPACITY	Horizon
Organic Carbon Content (%)	ORGANIC CARBON	Horizon
Application Mass, Chemical 1 (kg/ha)	APPLICATION 1	Application
Application Mass, Chemical 2 (kg/ha)	APPLICATION 2	Application
Application Mass, Chemical 3 (kg/ha)	APPLICATION 3	Application
Dispersion Coeff., Chemical 1 (cm^2/day)	DISPERSION 1	Horizon
Dispersion Coeff., Chemical 2 (cm^2/day)	DISPERSION 2	Horizon
Dispersion Coeff., Chemical 3 (cm^2/day)	DISPERSION 3	Horizon
Decay Rate in Water, Chemical 1 (days^{-1})	WATER DECAY 1	Horizon
Decay Rate in Water, Chemical 2 (days^{-1})	WATER DECAY 2	Horizon
Decay Rate in Water, Chemical 3 (days^{-1})	WATER DECAY 3	Horizon
Decay Rate of Vapor, Chemical 1 (days^{-1})	VAPOR DECAY 1	Horizon
Decay Rate of Vapor, Chemical 2 (days^{-1})	VAPOR DECAY 2	Horizon
Decay Rate of Vapor, Chemical 3 (days^{-1})	VAPOR DECAY 3	Horizon
Decay Rate of Sorbed Chemical 1 (days^{-1})	SORBED DECAY 1	Horizon
Decay Rate of Sorbed Chemical 2 (days^{-1})	SORBED DECAY 2	Horizon
Decay Rate of Sorbed Chemical 3 (days^{-1})	SORBED DECAY 3	Horizon
Henry's Constant, Chemical 1	HENRY'S CONSTANT 1	--
Henry's Constant, Chemical 2	HENRY'S CONSTANT 2	--
Henry's Constant, Chemical 3	HENRY'S CONSTANT 3	--
Irrigation Moisture Level (Fraction)	IRRIG LEVEL	--
Application Year	APP YEAR	Application
Julian Application Day	APP DAY	Application

TABLE 4-7. MONTE CARLO LABELS FOR PRZM VARIABLES (concluded)

Parameter	Monte Carlo Label	Index
Model Outputs		
Soil Water Content (cm^3/cm^3)	THETA	Compartment
Total Soil Pesticide, Chemical 1 (kg/ha)	SOIL PESTICIDE 1	Compartment
Total Soil Pesticide, Chemical 2 (kg/ha)	SOIL PESTICIDE 2	Compartment
Total Soil Pesticide, Chemical 3 (kg/ha)	SOIL PESTICIDE 3	Compartment
Infiltration Depth (cm)	INFILTRATION	--
Runoff depth (cm)	RUNOFF	--
Precipitation (cm)	PRECIPITATION-	-
Evapotranspiration (cm)	EVAPOTRANSPIRATION	Compartment
Flood or Furrow Irrigation Depth	IRRIG DEPTH	--
Runoff Flux, Chemical 1 (kg/ha/day)	RUNOFF FLUX 1	--
Runoff Flux, Chemical 2 (kg/ha/day)	RUNOFF FLUX 2	--
Runoff Flux, Chemical 3 (kg/ha/day)	RUNOFF FLUX 3	--
Erosion Flux, Chemical 1 (kg/ha/day)	EROSION FLUX 1	--
Erosion Flux, Chemical 2 (kg/ha/day)	EROSION FLUX 2	--
Erosion Flux, Chemical 3 (kg/ha/day)	EROSION FLUX 3	--
Decay Flux, Chemical 1 (kg/ha/day)	DECAY FLUX 1	Compartment
Decay Flux, Chemical 2 (kg/ha/day)	DECAY FLUX 2	Compartment
Decay Flux, Chemical 3 (kg/ha/day)	DECAY FLUX 3	Compartment
Volat. Flux, Chemical 1 (kg/ha/day)	VOLAT. FLUX 1	Compartment
Volat. Flux, Chemical 2 (kg/ha/day)	VOLAT. FLUX 2	Compartment
Volat. Flux, Chemical 3 (kg/ha/day)	VOLAT. FLUX 3	Compartment
Plant Flux, Chemical 1 (kg/ha/day)	PLANT FLUX 1	Compartment
Plant Flux, Chemical 2 (kg/ha/day)	PLANT FLUX 2	Compartment
Plant Flux, Chemical 3 (kg/ha/day)	PLANT FLUX 3	Compartment
Root Zone Flux, Chemical 1 (kg/ha/day)	ROOT FLUX 1	--
Root Zone Flux, Chemical 2 (kg/ha/day)	ROOT FLUX 2	--
Root Zone Flux, Chemical 3 (kg/ha/day)	ROOT FLUX 3	--

Table 4-8. MONTE CARLO LABELS FOR VADOFT VARIABLES

Parameter	Monte Carlo Label	Index
Random Model Inputs		
Hydraulic Conductivity	HYDRAULIC CONDUC	Material
Residual Saturation	RESIDUAL SATURATION	Material
Van-Genuchten Alpha	V-G ALPHA	Material
Van-Genuchten N	V-G POWER N	Material
Decay Rate Chemical 1	VADOFT DECAY 1	Material
Decay Rate Chemical 2	VADOFT DECAY 2	Material
Decay Rate Chemical 3	VADOFT DECAY 3	Material
Dispersion Coefficient, Chemical 1	VAD DISPC 1	Material
Dispersion Coefficient, Chemical 2	VAD DISPC 2	Material
Dispersion Coefficient, Chemical 3	VAD DISPC 3	Material
Retardation, Chemical 1	VAD RETARD 1	Material
Retardation, Chemical 2	VAD RETARD 2	Material
Retardation, Chemical 3	VAD RETARD 3	Material
Model Outputs (Note: Fluxes are net fluxes for the entire soil column)		
Total Water Flux	VAD WATER FLUX	--
Advective Flux, Chemical 1	VAD ADVECTION 1	--
Advective Flux, Chemical 2	VAD ADVECTION 2	--
Advective Flux, Chemical 3	VAD ADVECTION 3	--
Dispersion Flux, Chemical 1	VAD DISPERSION 1	--
Dispersion Flux, Chemical 2	VAD DISPERSION 2	--
Dispersion Flux, Chemical 3	VAD DISPERSION 3	--
Decay Flux, Chemical 1	VAD DECAY FLUX 1	--
Decay Flux, Chemical 2	VAD DECAY FLUX 2	--
Decay Flux, Chemical 3	VAD DECAY FLUX 3	--
Concentration, Chemical 1	VAD CONC 1	Node
Concentration, Chemical 2	VAD CONC 2	Node
Concentration, Chemical 3	VAD CONC 3	Node

Table 4-9. MONTE CARLO LABELS FOR SAFTMOD VARIABLES

Parameter	Monte Carlo Label	Index
Random Model Inputs		
Hydraulic Conductivity KXX	KXX	Material
Hydraulic Conductivity KYY	KYY	Material
Longitudinal Dispersivity	LONG DISP	Mateiral
Transverse Dispersivity	TRANS DISP	Material
Chemical Decay Rate, Chemical 1	SAFT DECAY 1	Material
Chemical Decay Rate, Chemical 2	SAFT DECAY 2	Material
Chemical Decay Rate, Chemical 3	SAFT DECAY 3	Material
Retardation Coeff., Chemical 1	SAFT RETARD 1	Material
Retardation Coeff., Chemical 2	SAFT RETARD 2	Material
Retardation Coeff., Chemical 3	SAFT RETARD 3	Material
Model Outputs (Note: Fluxes are net fluxes for the entire SAFTMOD grid)		
Total Water Flux	SAFT WATER FLUX	--
Advective Flux, Chemical 1	SAFT ADVECTION 1	--
Advective Flux, Chemical 2	SAFT ADVECTION 2	--
Advective Flux, Chemical 3	SAFT ADVECTION 3	--
Dispersion Flux, Chemical 1	SAFT DISPERSION 1	--
Dispersion Flux, Chemical 2	SAFT DISPERSION 2	--
Dispersion Flux, Chemical 3	SAFT DISPERSION 3	--
Decay Flux, Chemical 1	SAFT DECAY FLUX 1	--
Decay Flux, Chemical 2	SAFT DECAY FLUX 2	--
Decay Flux, Chemical 3	SAFT DECAY FLUX 3	--
Concentration, Chemical 1	SAFT CONC 1	Node
Concentration, Chemical 2	SAFT CONC 2	Node
Concentration, Chemical 3	SAFT CONC 3	Node

correlated. The third entry on these data lines is the value of the correlation coefficient. After a data line is supplied for each correlated pair of parameters, an END card must be provided to mark the end of the data group.

RECORD 7. PNAME(1), INDI1, INDZ1, PNAME(2), INDI2, INDZ2, CORR(1,2)

FORMAT(2(A20, 2I5), F10.0)

PNAME(1): A 1- to 20-character label identifying the first correlated parameter. Distribution type must be normal, log-normal, Johnson SU, or Johnson SB.

INDI1: The array index for the first parameter (see Tables 4.7, 4.8 and 4.9).

INDZ1: The aquifer number for the first parameter (SAFTMOD variables only). Leave blank for PRZM and VADOFT variables.

PNAME(2): A 1- to 20-character label identifying the second correlated parameter. Distribution type must be normal, log-normal, Johnson SU, or Johnson SB.

INDI2: The array index for the second parameter (see Tables 4.7, 4.8 and 4.9).

INDZ2: The aquifer number for the second parameter (SAFTMOD variables only). Leave blank for PRZM and VADOFT variables.

CORR(1,2): The value of the correlation coefficient for parameters 1 and 2.

SECTION 5

PARAMETER ESTIMATION

This section describes procedures and provides information to aid the user of RUSTIC in estimating model input parameters. Parameters in each of the modules are covered beginning with the Executive Supervisor (5.1), PRZM (5.2), VADOFT (5.3), and SAFTMOD (5.4).

5.1 EXECUTION SUPERVISOR

The execution supervisor does not have any parameters per se. The input data stream to the execution supervisor is composed of what options are selected, file names, and global data. The global data consists of the start and ending dates of the current simulation, the number of days per SAFTMOD simulation (required only if the SAFTMOD option is selected), the number of chemicals which will be simulated (if solute transport is being simulated), and the index of the parent species of each solute being simulated (required only if solute transport is being simulated and the number of chemicals being simulated is greater than one).

With the exception of the parameter defining the number of days in a SAFTMOD simulation, the values selected for the execution supervisor input stream result from the definition of the problem being simulated. A reasonable value of the SAFTMOD time step can be determined from examining the grid spacing and expected velocities in the saturated zone.

The number of days in a SAFTMOD simulation can be as small as one and as large as the total number of days being simulated. Lower values of this parameter will increase accuracy and also increase the execution time (restart data have to be read from disk files each time a new SAFTMOD simulation is started). The most accurate simulations will be obtained by defining the time step such that water will move, on the average, across one SAFTMOD element each time step. The water velocity can be estimated by multiplying the head gradient times the hydraulic conductivity. Dividing the average SAFTMOD element length by this velocity estimate will provide an estimate of the time step.

5.2 PRZM PARAMETERS

With a few exceptions, PRZM Release II has the same parameter requirements as PRZM Release I (Carsel et al. 1984). This section contains guidance for original PRZM parameters, extracted from the original report, as well as additional parameters required by the addition of several new capabilities. New capabilities include:

- Volatilization
- Daughter Products Simulation
- Soil Temperature Simulation

PRZM relates pesticide fate in the upper soil to temporal variations in hydrologic, agronomic, and pesticide chemical factors. A minimum of generally accessible input is required for successful use of PRZM. The module does utilize some parameters, however, that users may find difficult to obtain or calculate. The following sections describe these parameters and provide detailed procedures for estimating or obtaining the required values. In addition, where information was available, coefficients of variation (CV) and distribution type are provided for use with Monte Carlo simulation. Parameters appear in the same general order that they appear in the input file. Options are available in the program to directly estimate several parameters (e.g., soil water content at field capacity, wilting point, bulk density, adsorption partition coefficients, soil thermal conductivity, heat capacity), when related information is supplied by the user.

5.2.1 Hydrology Parameters

SFAC and PFAC--Snow Factor and Pan Factor--
When the mean air temperature (T) falls below 0.0°C, any precipitation that falls is considered to be in the form of snow. When the mean air temperature is above 0.0°C, however, the snow accumulation is decreased by a snowmelt factor, SFAC. The amount of snowmelt is calculated by the degree-day factor and was described in Section 2 (Volume I). The mean air temperature is read from the meteorological file.

The snowmelt factor, SFAC, usually increases as forest cover decreases; typical minimum and maximum ranges for SFAC for different forest cover conditions are provided in Table 5-1. Climatic and physiographic factors will have an effect on values selected for site-specific conditions. Higher values of SFAC are appropriate for sites with windy conditions and where south-facing slopes are predominant (Anderson 1978). The snow factor would be applicable only to those areas where the climatology produces temperatures conducive to snow fall and snow melt.

The pan factor (PFAC) is a dimensionless number used to convert daily pan evaporation to daily potential ET. The pan factor generally ranges between 0.60-0.80. Figure 5.1 illustrates typical pan factors in specific regions of the United States.

ANETD--Soil Evaporation Moisture Loss During Fallow, Dormant Periods--
The soil water balance model considers both soil evaporation and plant transpiration losses and updates the depth of water extraction by plant roots during the growing season. The total evapotranspiration demand (ET) is subtracted sequentially in a linearly weighted manner from each layer until a minimum moisture level (wilting point) is reached within each layer. Evaporation is initially assumed to occur in the top 10 cm of the soil profile with the remaining demand, crop transpiration, occurring from compartments below the 10-cm zone and down to the maximum depth of rooting.

Table 5-1. TYPICAL VALUES OF SNOWMELT FACTOR (SFAC) AS RELATED TO FOREST COVER

Forest Cover	Snowmelt Factor, SFAC (cm °C^{-1} day^{-1}) Minimum	Snowmelt Factor, SFAC (cm °C^{-1} day^{-1}) Maximum
Coniferous forest - quite dense	0.08 - 0.12	0.20 - 0.32
Mixed forest - coniferous plus open areas and/or deciduous	0.10 - 0.16	0.32 - 0.40
Predominantly deciduous forest	0.14 - 0.20	0.40 - 0.52
Open areas	0.20 - 0.36	0.52 - 0.80

Source: Anderson, E.A., "Initial Parameter Values for the Snow Accumulation and Ablation Model", Part IV.2.2.1, National Weather Service River Forecast System - User's Manual, NWS/NOAA, U.S. Dept. of Commerce, Silver Springs, MD, March 31, 1978.

These assumptions allow simulation of reduced levels of ET during fallow, dormant periods and increased levels during active plant growth. Values for (ANETD) used to estimate soil evaporation losses are provided in Figure 5.2.

The values for ANETD in Figure 5.2 are only applicable for soil hydraulics option 1, the free drainage model, and would not be appropriate for use with hydraulics option 2, the limited drainage model. The limited drainage model allows more available soil water and, hence, more ET extraction. If drainage option 2 is selected, it is recommended that ANETD be set to equal 10 cm. Calibration may be required if results are not consistent with local water balance data.

DT--Average Day Time Hours for a Day in Each Month--
The values of DT are used to calculate total potential ET using Hamon's Formula if daily pan evaporation data do not exist. Values of DT for latitudes 0 - 50° north or south of the equator are provided in Table 5-2.

Values for DT are determined by:

Step 1. Finding the approximate degree latitude north or south of the equator for the location.

Step 2. Inputting the twelve monthly numbers under the degree latitude column into the parameter file in calendar order, i.e., January through December.

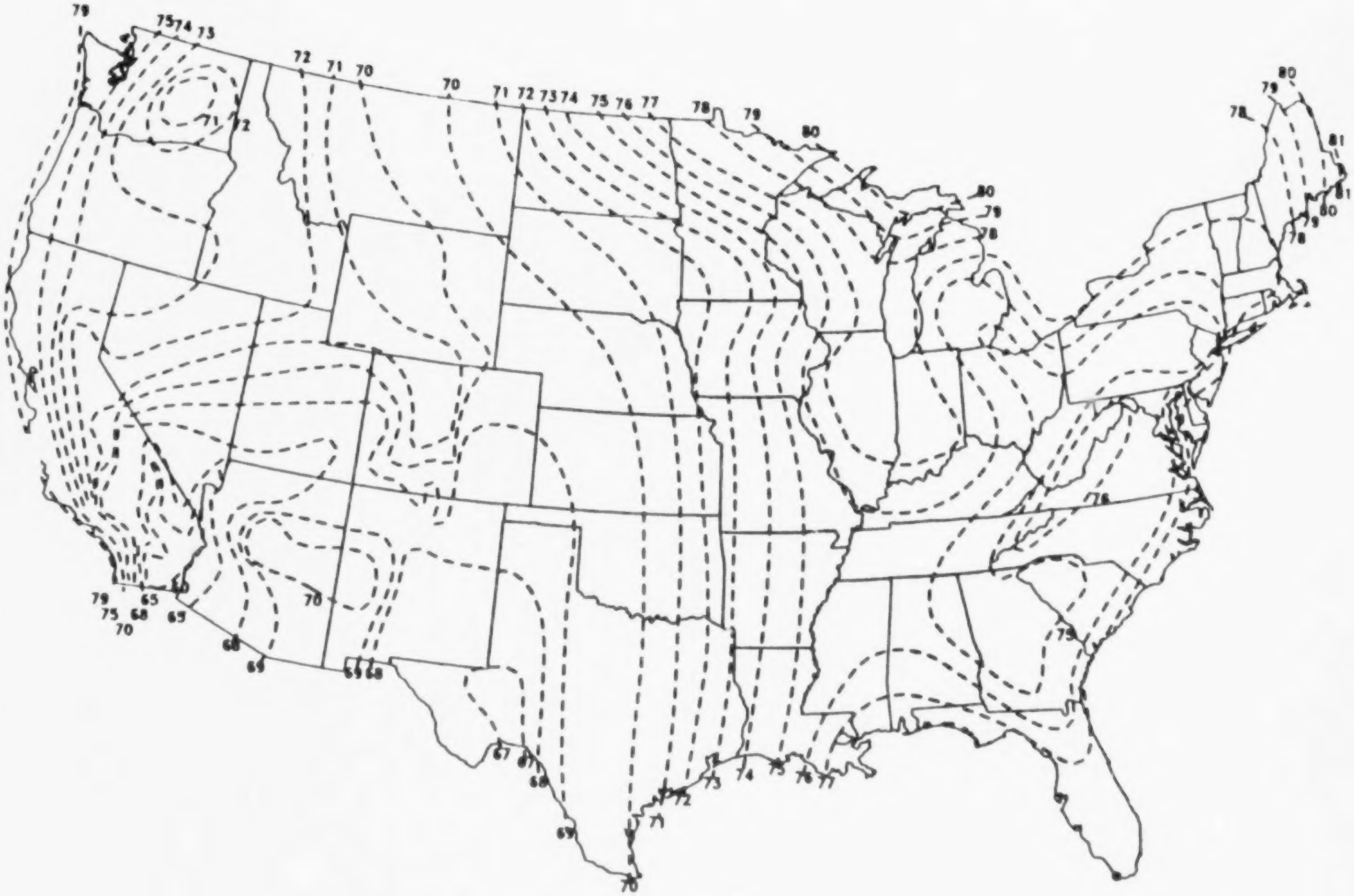

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Figure 5.1. Pan evaporation correction factors (from U.S. Weather Bureau).

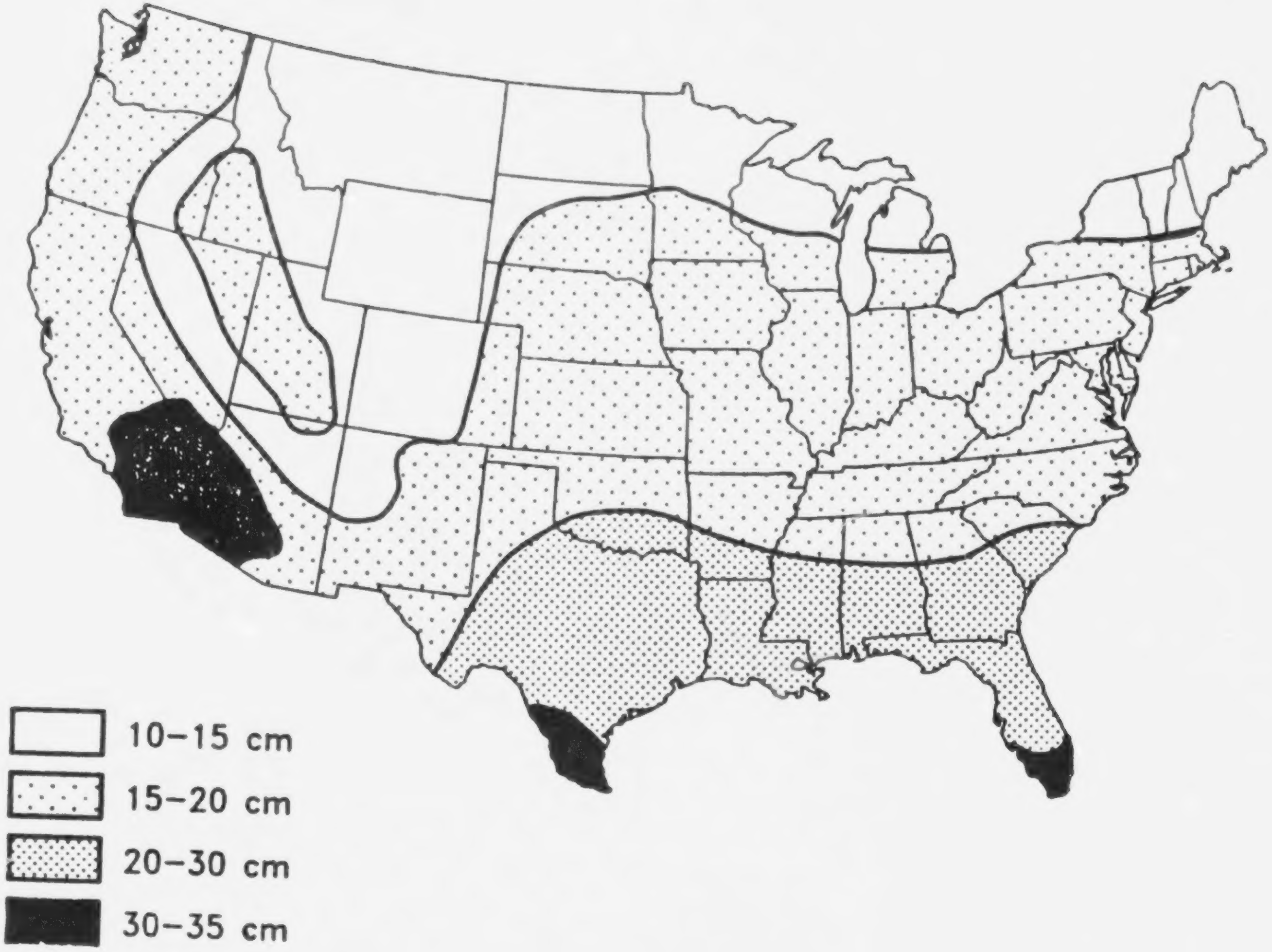
10–15 cm
15–20 cm
20–30 cm
30–35 cm

Figure 5.2. Diagram for estimating soil evaporation loss.

Table 5-2. MEAN DURATION (HOURS) OF SUNLIGHT FOR LATITUDES 0° TO 50° IN THE NORTHERN AND SOUTHERN HEMISPHERES[a]

	Month of the Year[b]												
Latitude*	Jan Jul	Feb Aug	Mar Sep	Apr Oct	May Nov	Jun Dec	Jul Jan	Aug Feb	Sep Mar	Oct Apr	Nov May	Dec Jun	(N.H.) (S.H.)
0	12.5	11.3	12.5	12.1	12.5	12.7	12.5	12.5	12.1	12.5	12.1	12.5	
10	12.0	10.9	12.4	12.4	13.0	12.7	13.0	12.8	12.2	12.2	11.8	11.9	
20	11.4	10.8	12.4	12.6	13.6	13.3	13.7	13.3	12.2	12.0	11.2	11.3	
30	10.8	10.4	12.4	13.0	14.2	14.0	14.4	13.7	12.4	11.8	10.7	10.6	
35	10.4	10.2	12.4	13.1	14.5	14.5	14.8	13.9	12.4	11.6	10.3	10.2	
40	10.1	10.0	12.4	13.3	14.9	15.0	15.2	14.2	12.5	11.5	10.0	9.7	
45	9.6	9.7	12.2	13.6	15.4	15.5	15.7	14.5	12.5	11.3	9.5	9.0	
50	8.9	9.4	12.2	13.8	16.0	16.3	16.4	15.0	12.7	11.0	9.1	8.4	

a - Criddle, W.D. Methods of Computing Consumptive Use of Water, Proceedings ASCE. 84(IR 1). 1958.

b - Values for the southern hemisphere were assumed equal to northern hemisphere values lagged by six months, e.g., the duration for January in the northern hemisphere is the same as July in the southern hemisphere.

* - Degrees North or South of Equator

N.H. - Northern Hemisphere
S.H. - Southern Hemisphere

Example: 40° north latitude
10.1, 10.0, 12.4, 13.3, 14.9, 15.0,
15.2, 14.2, 12.5, 11.5, 10.0, 9.7

USLEK, USLELS, USLEP, USLEC--Universal Soil Loss Equation Parameters--
The role of erosion on pesticide loss decreases with decreasing chemical affinity for soil. The total mass of pesticide loss by this means for most highly soluble pesticides will be quite small. If the apparent distribution coefficient is less or equal to 5.0, erosion can usually be neglected (i.e., the erosion flag ERFLAG can be set to zero). For a compound having a distribution coefficient greater than 5.0, erosion losses (and subsequent pesticide loss) should be estimated and the erosion flag set (to one) accordingly.

Soil characteristics, climatic conditions, agronomic practices, and topography contribute to the potential erosion rate from a field. During an erosion-producing runoff event, soil particles and aggregates are carried across the field. These aggregates consist of coarse, medium, and fine particles, with the finer particles carried the greatest distances across the field. Sediment is the principal carrier of sorbed pesticides.

The Universal Soil Loss Equation (USLE) developed by USDA is a simple method used to determine erosion losses. The USLE is most accurate for long-term average erosion losses. The soil loss equation used in PRZM uses the modification described by Williams (1975). The Williams modification replaces the R (rainfall erosivity) term with an energy term. The energy term enables the estimation of event totals for erosion from the field. The modified universal soil loss equation (MUSLE) requires the remaining four USLE factors with no modifications.

USLEK--Soil Erodibility Factor--
USLEK is a soil specific parameter. Specific values for various soils are obtainable from local Soil Conservation Service (SCS) offices. Approximate values (based on broad ranges of soil properties) can be estimated from Table 5-3.

USLELS--Slope Length and Steepness Factor--
USLELS is a topographic parameter and is dimensionless. Values for LS can be estimated from Table 5-4.

USLEP--Supporting Practice Factor--
USLEP is a conservation supporting practice parameter and is dimensionless. Values range from 0.10 (extensive practices) to 1.0 (no supporting practice). Specific values for P can be estimated from Table 5-5.

USLEC--Cover and Management Factor--
USLEC is a management parameter and is dimensionless. Values range from 0.001 (well managed) to 1.0 (fallow or tilled condition). One value for each of the three growing periods (fallow, cropping, residue) is required. Specific local values can be computed from Wischmeier and Smith (1978) or obtained from the local SCS office. Generalized values are provided in Table 5-6.

Table 5-3. INDICATIONS OF THE GENERAL MAGNITUDE OF THE SOIL/ERODIBILITY FACTOR, K[a]

Texture Class	Organic Matter Content		
	<0.5%	2%	4%
Sand	0.05	0.03	0.02
Fine Sand	0.16	0.14	0.10
Very fine sand	.42	.36	.28
Loamy sand	.12	.10	.08
Loamy fine sand	.24	.20	.16
Loamy very fine sand	.44	.38	.30
Sandy loam	.27	.24	.19
Fine sandy loam	.35	.30	.24
Very fine sandy loam	.47	.41	.33
Loam	.38	.34	.29
Silt loam	.48	.42	.33
Silt	.60	.52	.42
Sandy clay loam	.27	.25	.21
Clay loam	.28	.25	.21
Silty clay loam	.37	.32	.26
Sandy clay	.14	.13	.12
Silty clay	.25	.23	.19
Clay		0.13-0.29	

[a] The values shown are estimated averages of broad ranges of specific-soil values. When a texture is near the borderline of two texture classes, use the average of the two K values. For specific soils, Soil Conservation Service K-value tables will provide much greater accuracy. (Control of Water Pollution from Cropland, Vol. I, A Manual for Guideline Development. U.S. Environmental Protection Agency, Athens, GA EPA-600/2-75-026a).

Table 5-4. VALUES OF THE EROSION EQUATION'S TOPOGRAPHIC FACTOR, LS, FOR SPECIFIED COMBINATIONS OF SLOPE LENGTH AND STEEPNESS[a]

% Slope	Slope Length (feet)											
	25	50	75	100	150	200	300	400	500	600	800	100
0.5	0.07	0.08	0.09	0.10	0.11	0.12	0.14	0.15	0.16	0.17	0.19	0.20
1	0.09	0.10	0.12	0.13	0.15	0.16	0.18	0.20	0.21	0.22	0.24	0.26
2	0.13	0.16	0.19	0.20	0.23	0.25	0.28	0.30	0.33	0.34	0.38	0.40
3	0.19	0.23	0.26	0.29	0.33	0.35	0.40	0.44	0.47	0.49	0.54	0.57
4	0.23	0.30	0.36	0.40	0.47	0.53	0.62	0.70	0.76	0.82	0.92	1.0
5	0.27	0.38	0.46	0.54	0.66	0.76	0.93	1.1	1.2	1.3	1.4	1.7
6	0.34	0.48	0.58	0.67	0.82	0.95	1.2	1.4	1.5	1.7	1.9	2.1
8	0.50	0.70	0.86	0.99	1.2	1.4	1.7	2.0	2.2	2.4	2.8	3.1
10	0.69	0.97	1.2	1.4	1.7	1.9	2.4	2.7	3.1	3.4	3.9	4.3
12	0.90	1.3	1.6	1.8	2.2	2.6	3.1	3.6	4.0	4.4	5.1	5.7
14	1.2	1.6	2.0	2.3	2.8	3.3	4.0	4.6	5.1	5.6	6.5	7.3
16	1.4	2.0	2.5	2.8	3.5	4.0	4.9	5.7	6.4	7.0	8.0	9.0
18	1.7	2.4	3.0	3.4	4.2	4.9	6.0	6.9	7.7	8.4	9.7	11.0
20	2.0	2.9	3.5	4.1	5.0	5.8	7.0	8.2	9.1	10.0	12.0	13.0
25	3.0	4.2	5.1	5.9	7.2	8.3	10.0	12.0	13.0	14.0	17.0	19.0
30	4.0	5.6	6.9	8.0	9.7	11.0	14.0	16.0	18.0	20.0	23.0	25.0
40	6.3	9.0	11.0	13.0	16.0	18.0	22.0	25.0	28.0	31.0	--	--
50	8.9	13.0	15.0	18.0	22.0	25.0	31.0	--	--	--	--	--
60	12.0	16.0	20.0	23.0	28.0	--	--	--	--	--	--	--

---

[a] Values given for slopes longer than 300 feet or steeper than 18% are extrapolations beyond the range of the research data, and therefore, less certain than the others. (Control of Water Pollution from Cropland, Vol. I, A Manual for Guideline Development. U.S. Environmental Protection Agency, Athens, GA. EPA-600/275-026a).

Table 5-5. VALUES OF SUPPORT-PRACTICE FACTOR, P[a]

Practice	Land Slope (percent)				
	1.1-2.0	2.1-7.0	7.1-12.0	12.1-18.0	18.1-24.0
			(Factor P)		
Contouring (P_c)	0.60	0.50	0.60	0.80	0.90
Contour Strip cropping (P_{sc})[b]					
R-R-M-M	0.30	0.25	0.30	0.40	0.45
R-W-M-M	0.30	0 25	0.30	0.40	0.45
R-R-W-M	0.45	0.38	0.45	0.60	0.68
R-W	0.52	0.44	0.52	0.70	0.90
R-O	0.60	0.50	0.60	0.80	0.90
Contour listing or ridge planting (P_{cl})	0.30	0.25	0.30	0.40	0.45
Contour terracing (P_t)[c]	[d]$0.6/\sqrt{n}$	$0.5/\sqrt{n}$	$0.6/\sqrt{n}$	$0.8/\sqrt{n}$	$0.9/\sqrt{n}$
No support practice	1.0	1.0	1.0	1.0	1.0

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[a] Control of Water Pollution from Cropland, Vol. I, A Manual for Guideline Development. U.S. Environmental Protection Agency, Athens, GA. EPA-600/2-75-026a.

[b] R = rowcrop, W = fall-seeded grain, O = spring-seeded grain, M = meadow. The crops are grown in rotation and so arranged on the field that rowcrop strips are always separated by a meadow or winter-grain strip.

[c] These P_t values estimate the amount of soil eroded to the terrace channels and are used for conservation planning. For prediction of off-field sediment, the P_t values are multiplied by 0.2.

[d] n = number of approximately equal-length intervals into which the field slope is divided by the terraces. Tillage operations must be parallel to the terraces.

Table 5-6. GENERALIZED VALUES OF THE COVER AND MANAGEMENT FACTOR, C, IN THE 37 STATES EAST OF THE ROCKY MOUNTAINS[a,b]

Line No.	Crop, Rotation, and Management[c]	Productivity Level[d] High	Productivity Level[d] Mod.
		C Value	C Value
	Base value: continuous fallow, tilled up and down slope	1.00	1.00
	Corn		
1	C, RdR, fall TP, conv (1)	0.54	0.62
2	C, RdR, spring TP, conv (1)	.50	.59
3	C, RdL, fall TP, conv (1)	.42	.52
4	C, RdR, wc seeding, spring TP, conv (1)	.40	.49
5	C, RdL, standing, spring TP, conv (1)	.38	.48
6	C, fall shred stalks, spring TP, conv (1)	.35	.44
7	C(silage)-W(RdL, fall TP) (2)	.31	.35
8	C, RdL, fall chisel, spring disk, 40-30% rc (1)	.24	.30
9	C(silage), W wc seeding, no-till pl in c-k (1)	.20	.24
10	C(RdL)-W)RdL, spring TP) (2)	.20	.28
11	C, fall shred stalks, chisel pl, 40-30% rc (1)	.19	.26
12	C-C-C-W-M, RdL, TP for C, disk for W (5)	.17	.23
13	C, RdL, strip till row zones, 55-40% rc (1)	.16	.24
14	C-C-C-W-M-M, RdL, TP for C, disk for W (6)	.14	.20
15	C-C-W-M, RdL, TP for C, disk for W (4)	.12	.17
16	C, fall shred, no-till pl, 70-50% rc (1)	.11	.18
17	C-C-W-M-M, RdL, TP for C, disk for W (5)	.087	.14
18	C-C-C-W-M, RdL, no-till pl 2nd & 3rd C (5)	.076	.13
19	C-C-W-M, RdL, no-till pl 2d C (4)	.068	.11
20	C, no-till pl in c-k wheat, 90-70% rc (1)	.062	.14
21	C-C-C-W-M-M, no-till pl 2d & 3rd C (6)	.061	.11
22	C-W-M, RdL, TP for C, disk for W (3)	.055	.095
23	C-C-W-M-M, RdL, no-till pl2d C (5)	.051	.094
24	C-W-M-M, RdL, TP for C, disk for W (4)	.039	.074
25	C-W-M-M-M, RdL, TP for C, disk for W (5)	.032	.061
26	C, no-till pl in c-k sod, 95-80% rc (1)	.017	.053
	Cotten[e]		
27	Cot, conv (Western Plains) (1)	0.42	0.49
28	Cot, conv (South) (1)	.34	.40
	Meadow		
29	Grass & Legume mix	0.004	0.01
30	Alfalfa, lespedeza or Sericia	.020	
31	Sweet clover	.025	

Table 5-6. GENERALIZED VALUES OF THE COVER AND MANAGEMENT FACTOR, C, IN THE 37 STATES EAST OF THE ROCKY MOUNTAINS[a,b] (continued)

Line No.	Crop, Rotation, and Management[c]	Productivity Level[d] High	Productivity Level[d] Mod.
		C Value	C Value
Base value:	continuous fallow, tilled up and down slope	1.00	1.00
Sorghum, grain (Western Plains)[e]			
32	RdL, spring TP, conv (1)	0.43	0.53
33	No-till pl in shredded 70-50% rc	.11	.18
Soybeans[e]			
34	B, RdL, spring TP, conv (1)	0.48	0.54
35	C-B, TP annually, conv (2)	.43	.51
36	B, no-till pl	.22	.28
37	C-B, no-till pl, fall shred C stalks (2)	.18	.22
Wheat			
38	W-F, fall TP after W (2)	0.38	
39	W-F, stubble mulch, 500 lbs rc (2)	.32	
40	W-F, stubble mulch, 1000 lbs rc (2)	.21	
41	Spring W, RdL, Sept TP, conv (N&S Dak) (1)	.23	
42	Winter W, RdL, Aug TP, conv (Kansas) (1)	.19	
43	Spring W, stubble mulch, 750 lbs rc (1)	.15	
44	Spring W, stubble mulch, 1250 lbs rc (1)	.12	
45	Winter W, stubble mulch, 750 lbs rc (1)	.11	
46	Winter W, stubble mulch, 1250 lbs rc (1)	.10	
47	W-M, conv (2)	.054	
48	W-M-M, conv (3)	.026	
49	W-M-M-M, CONV (4)	.021	

---

[a] This table is for illustrative purposes only and is not a complete list of cropping systems or potential practices. Values of C differ with rainfall pattern and planting dates. These generalized values show approximately the relative erosion-reducing effectiveness of various crop systems, but locationally derived C values should be used for conservation planning at the field level. Tables of local values are available from the Soil Conservation Service.

[b] Control of Water Pollution from Cropland, Vol. I, A Manual for Guide-line Development. U.S. Environmental Protection Agency, Athens, GA. EPA-600/3-75-026a.

[c] Numbers in parentheses indicate number of years in the rotation cycle. No. (1) designates a continous one-crop system.

[d] High level is exemplified by long-term yield averages greater than 75 bu. corn or 3 tons grass-and-legume hay; or cotton management that regularly provides good stands and growth.

Table 5-6. GENERALIZED VALUES OF THE COVER AND MANAGEMENT FACTOR, C, IN THE 37 STATES EAST OF THE ROCKY MOUNTAINS[a,b] (concluded)

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[e] Grain sorghum, soybeans, or cotton may be substituted for corn in lines 12, 14, 15, 17-19, 21-25 to estimate C values for sod-based rotations.

Abbreviations defined:

B	- soybeans	F	- fallow
C	- corn	M	- grass & legume hay
c-k	- chemically killed	pl	- plant
conv	- conventional	W	- wheat
cot	- cotton	we	- cover
lbs rc	- pounds of crop residue per acre remaining on surface after new crop seeding		
% rc	- percentage of soil surface covered by residue mulch after new crop seeding		
70-50% rc	- 70% cover for C values in first column; 50% for second column		
RdR	- residues (corn stover, straw, etc.) removed or burned		
RdL	- all residues left on field (on surface or incorporated)		
TP	- turn plowed (upper 5 or more inches of soil inverted, covering residues)		

TR--Storm Duration--Peak Runoff Rate--
Total runoff is easily calculated with the curve number technique, but the problem remains to estimate the peak runoff rate. Most runoff producing storms occur over a short duration. The model assumes a trapezoidal hydrograph (see Section 2, Vol. I) with storm duration (TR) specified as an input. Unfortunately, data to estimate TR are not often readily available.

TR is entered as an average, although in reality this parameter changes seasonally as well as with individual storm type. Because most erosion losses occur shortly after plowing or other tillage prior to crop emergence, the value of TR should be appropriate for this period. Several references (Heimstra and Crease, 1970; Grace and Eagleson 1966; Varas and Linsley, 1977; Eagleson, 1978; and Dean, 1979) give representative values of storm duration. Table 5-7 provides estimates of TR for selected locations in the United States for both mean annual and summer time periods, while Figure 5.3 provides "regionalized" values for different areas of the U.S. If more detailed site-specific information is desired, representative storm durations can be estimated from analysis of hourly rainfall records. Soil loss estimates can be adjusted by calibrating this parameter to match annual soil loss estimates. The soil loss estimates are proportional to $1/\sqrt{TR}$ (a four-fold decrease in TR will produce a two-fold increase in soil loss).

CINTCP--Maximum Crop Interception--
The crop interception parameter (CINTCP) estimates the amount of rainfall that is intercepted by a fully developed plant canopy and retained on the plant surface, cm. A range of 0.1 - 0.3 cm for a dense crop canopy is reported USDA (1980). Values for several major crops are provided in Table 5-8.

AMXDR--Active Crop Rooting Depth--
PRZM requires input of the maximum active crop rooting depth (AMXDR), in centimeters, for the simulated crop (or the deepest root zone of multiple crop simulations) measured from the land surface. Generalized information for corn, soybeans, wheat, tobacco, grain sorghum, potatoes, peanuts, and cotton are provided in Table 5-9. If minor crops, such as mint, are simulated, or site specific information alters the generalized information, consulting with USDA Handbook No. 283 (Usual Planting and Harvesting Dates), or the Cooperative Extension Service in the specific locale is advisable.

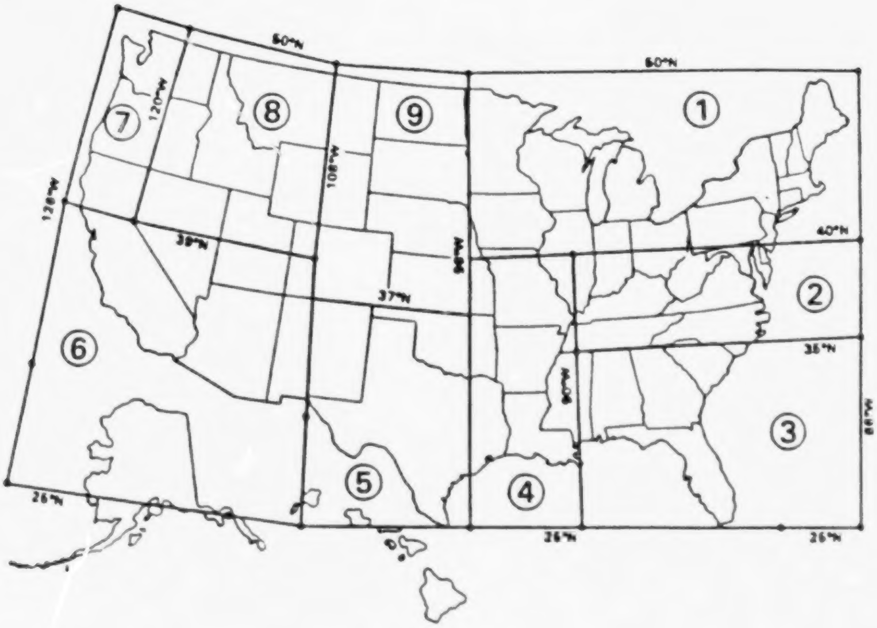
CN--Runoff Curve Number--
The interaction of hydrologic soil group (soil) and land use and treatment (cover) is accounted for by assigning a runoff curve number (CN) for average soil moisture condition (AMC II) to important soil cover complexes for the fallow, cropping, and residue parts of a growing season. The average curve numbers for each of the three soil cover complexes are estimated using Tables 5-10 through 5-14. The following steps provide a procedure for obtaining the correct curve numbers. Corn planted in straight rows will be used as an example.

Table 5-7. MEAN STORM DURATION* (TR) VALUES FOR SELECTED CITIES

	Storm Duration (hrs)	
Location	Mean Annual	Summer (June-Sept)
Great Lakes		
Champaign-Urbana, IL	6.1	4.6
Chicago, IL	5.7	4.5
Davenport, IA	6.6	5.3
Detroit, MI	4.4	3.1
Louisville, KY	6.7	4.5
Minneapolis, MN	6.0	4.5
Steubenville, OH	7.0	5.9
Toledo, OH	5.0	3.7
Zanesville, OH	6.1	4.3
Lansing, MI (30 Yr)	5.6	4.2
Lansing, MI (21 Yr)	6.2	5.1
Lower Mississippi Valley		
Memphis, TN	6.9	4.7
New Orleans, LA	6.9	5.0
Shreveport, LA (17 Yr)	7.8	5.3
Lake Charles, LA	7.7	5.9
Texas and Southwest		
Abilene, TX	4.2	3.3
Austin, TX	4.0	3.3
Brownsville, TX	3.5	2.8
Dallas, TX	4.2	3.2
El Paso, TX	3.3	2.6
Waco, TX	4.2	3.3
Phoenix, AZ	3.2	2.4
Northwest		
Portland, OR (25 Yr)	5.4	4.5
Portland, OR (10 Yr)	15.5	9.4
Eugene, OR	29.2	15.0
Seattle, WA	21.5	12.7
Southeast		
Greensboro, NC	5.0	3.6
Columbia, SC	4.5	3.4
Atlanta, GA	8.0	6.2
Birmingham, AL	7.2	5.0
Gainesville, FL	7.6	6.6
Tampa, FL	3.6	3.1
Rocky Mountains		
Denver, CO (8 Yr)	4.3	3.2
Denver, CO (25 Yr)	4.8	3.2
Denver, CO (24 Yr)	9.1	4.4
Rapid City, SD	8.0	6.1
Salt Lake City, UT	4.5	2.8
Salt Lake City, UT	7.8	6.8
California		
Oakland, CA	4.3	2.9
San Francisco, CA	5.9	11.2
Northeast		
Caribou, ME	5.8	4.4
Boston, MA	6.1	4.2
Lake George, NY	5.4	4.5
Kingston, NY	7.0	5.0
Poughkeepsie, NY	6.9	4.9
New York City, NY	6.7	4.8
Mineola, LI, NY	5.8	4.5
Upton LI, NY	6.3	4.6
Wantagh, LI, NY (2 Yr)	5.6	4.0
Long Island, NY	4.2	3.4
Washington, DC	5.9	4.1
Baltimore, MD	6.0	4.2

Source: Woodward-Clyde Consultants, "Methodology for Analysis of Detention Basins for Control of Urban Runoff Quality," prepared for U.S. EPA, Office of Water, Nonpoint Source Division, September, 1986.

* - These values may be misleading in arid regions or regions with pronounced seasonal rainfall patterns.


50°N
50°N
120°W
108°W
128°W
98°W
39°N
37°N
40°N
35°N
90°W
88°W
26°N
26°N
26°N
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MEAN STORM DURATION (hours)

	ZONE								
PERIOD	1	2	3	4	5	6	7	8	9
ANNUAL									
MEAN	5.8	5.9	6.2	7.3	4.0	3.6	20.0	4.5	4.4
C.V.	1.05	1.05	1.22	1.17	1.07	1.02	1.23	0.92	1.20
SUMMER									
MEAN	4.4	4.2	4.9	5.2	3.2	2.6	11.4	2.8	3.1
C.V.	1.14	1.09	1.33	1.29	1.08	1.01	1.20	0.80	1.14

Mean - mean value
C.V. - Coefficient of variation

Source: Woodward-Clyde Consultants, "Methodology for Analysis of Detention Basins for Control of Urban Runoff Quality", prepared for U.S. EPA, Office of Water, Nonpoint Source Division, September, 1986.

Figure 5.3. Representative regional mean storm duration (hours) values for the U.S.

Table 5-8. INTERCEPTION STORAGE FOR MAJOR CROPS

Crop	Density	CINTCP (cm)
Corn	Heavy	0.25 - 0.30
Soybeans	Moderate	0.20 - 0.25
Wheat	Light	0.0 - 0.15
Oats	Light	0.0 - 0.15
Barley	Light	0.0 - 0.15
Potatoes	Light	0.0 - 0.15
Peanuts	Light	0.0 - 0.15
Cotton	Moderate	0.20 - 0.25
Tobacco	Moderate	0.20 - 0.25

Step 1. From Appendix B of the users manual for PRZM, Release I (Carsel et al., 1984) or from Section 4 of the SCS National Engineering Handbook (Soil Conservation Service, 1972) find the hydrologic soil group for the particular soil that is in the area under consideration. There are four different soil classifications (A, B, C, and D), and they are in the order of decreasing percolation potential and increasing slope and runoff potential. Soil characteristics associated with each hydrologic group are as follows:

Group A: Deep sand, deep loess, aggregated silts, minimum infiltration of 0.76 - 1.14 (cm hr^{-1})

Group B: Shallow loess, sandy loam, minimum infiltration 0.38 - 0.76 (cm hr^{-1})

Group C: Clay loams, shallow sandy loam, soils low in organic content, and soils usually high in clay, minimum infiltration 0.13 - 0.38 (cm hr^{-1})

Group D: Soils that swell significantly when wet, heavy plastic clays, and certain saline soils, minimum infiltration 0.03 - 0.13 (cm hr^{-1})

If the soil series or soil properties are not known, the hydrologic soil group can be estimated from Figure 5.4.

Care must be exercised, however, in use of this figure. Considerable spatial aggregation was made in order to develop the generalized map over such a large area. Where possible, development of more highly resolved data is preferable.

Table 5-9. AGRONOMIC DATA FOR MAJOR AGRICULTURAL CROPS IN THE UNITED STATES

Crop	Representative States of Major States Production[a]	Planting Window, Month, Day (Julian Day)[b]	Crop Emergence (Days from Planting)	Crop Maturity (Days from Planting)	Harvest Window, Month, Day (Julian Day)[b]	Average Yield/Acre (1977-1979)[c]	Range of Active Plant Rooting Depth (cm)
Corn	IA, IL, IN NE, OH	April 25 (115) to June 15 (166)	5-15 5-15	110-130 110-130	Sept. 25 (268 to Dec. 10 (344)	110 bu	60-120
Soybeans	IA, IL, IN, MS, OH	May 1 (121) to June 25 (176)	5-15	110-130	Sept. 15 (258) to Dec. 10 (344)	35 bu	30-60
Cotton	TX, MS, CA, AZ, AR	March 1 (60) to May 25 (145) [TX to June 20 (171)]	5-15	110-130	Sept. 1 (244) to Jan. 15 (015) [TX Aug. 1 (213) to Dec. 20 (354)]	670 lbs	30-90
Wheat	KS, OK, CA, ND, MT, WA, MN, ID	Aug. 15 (227) to Oct. 25 (298) [WA to Nov. 20 (324), CA to Feb. 15 (046]	5-15	200-225	June 15 (166) to Sept. 20 (263)	40 bu	15-30
Potatoes	Long Island NY, ME, ID, WA, CA, OR	April 1 (091) to May 1 (121)	5-15	150-170	Sept. 1 (244) to Oct. 1 (274)	335 cwt	15-45
Peanuts	GA, TX, AL, NC, VA	April 5 (095) to June 5 (156) [TX Mar. 31 (090) to July 20 (201)]	5-15	150-175	Aug. 10 (222) to Dec. 15 (349)	2550 lbs	30-60
Tobacco	NC, SC, TN, KY, VA	April 5 (095) to June 20 (171)	Planted in Field as Seedling	120-150	July 1 (182) to Oct. 1 (274)	2000 lbs	30-60
Grain Sorghum	TX, KS, NE	TX Mar. 1 (060) to July 1 (182) KS, NE May 5 (125) to July 1 (182)	5-15	120-150	TX July 1 (182) to Nov. 20 (324) KS, NE Sept. 20 (263) to Dec. 1 (335)	62 bu	15-30

[a] Bay, D.M. and Bellinghausen, R.P. Missouri Farm Facts. Missouri Department of Agriculture. May 1979.

[b] Burkhead, B.E., Max, R.C., Karnes, R.B., and Neid, E. Usual Planting and Harvesting Dates. USDA, Agricultural Handbook No. 283. 1972.

[c] Kirkbride, J.W. (Ed.). Crop Production Annual Summary. USDA, Crop Reporting Board Publication CrPr 2-1. 1980.

Table 5-10. RUNOFF CURVE NUMBERS FOR HYDROLOGIC SOIL-COVER COMPLEXES[a] (ANTECEDENT MOISTURE CONDITION II, AND $I_a = 0.2$ S)

Cover			Hydrologic Soil Group			
Land Use	Treatment or Practice	Hydrologic Condition	A	B	C	D
Fallow	Straight Row	----	77	86	91	94
Row crops	Straight Row	Poor	72	78	85	91
	Straight row	Good	67	78	85	89
	Contoured	Poor	70	79	84	88
	Contoured	Good	65	75	82	86
	Contoured and terraced	Poor	66	74	80	82
	Contoured and terraced	Good	62	71	78	81
Small grain	Straight row	Poor	65	76	84	88
	Straight row	Good	63	75	83	87
	Contoured	Poor	63	74	83	87
	Contoured	Good	61	73	81	84
	Contoured and terraced	Poor	61	72	79	82
	Contoured and terraced	Good	59	70	78	81
Close-seeded legumes[b] or rotation meadow	Straight row	Poor	66	77	85	89
	Straight row	Good	58	72	81	85
	Contoured	Poor	64	75	83	85
	Contoured	Good	55	69	78	83
	Contoured and terraced	Poor	63	73	80	83
	Contoured and terraced	Good	51	67	76	80
Pasture or range		Poor	68	79	86	89
		Fair	49	69	79	84
		Good	39	61	74	80
	Contoured	Poor	47	67	81	88
	Contoured	Fair	25	59	75	83
	Contoured	Good	6	35	70	79
Meadow		Good	30	58	71	78
Woods		Poor	45	66	77	83
		Fair	36	60	73	79
		Good	25	55	70	77
Farmsteads		----	59	74	82	86
Roads (Dirt)[c]		----	72	82	87	89
(Hard Surface)[c]		----	74	84	90	92

[a] Mockus, 1972.
[b] Close-drilled or broadcast.
[c] Including right-of-way.

Table 5-11. METHOD FOR CONVERTING CROP YIELDS TO RESIDUE[a]

Crop[b]	Straw/Grain Ratio	Bushel Weight (lbs)
Barley	1.5	48
Corn	1.0	56
Oats	2.0	32
Rice	1.5	45
Rye	1.5	56
Sorghum	1.0	56
Soybeans	1.5	60
Winter wheat	1.7	60
Spring Wheat	1.3	60

[a] Crop residue = (straw/grain ratio) * (bushel weight in lb/bu) * (crop yield in bu/acre).

[b] Knisel, W.G. (Ed.). CREAMS: A Field-Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. USDA, Conservation Research Report No. 26, 1980.

Table 5-12. RESIDUE REMAINING FROM TILLAGE OPERATIONS[a]

Tillage[b] Operation	Residue Remaining (%)
Chisel Plow	65
Rod weeder	90
Light disk	70
Heavy disk	30
Moldboard plow	10
Till plant	80
Fluted coulter	90
V Sweep	90

[a] Crop residue remaining = (crop residue from Table 10) * (tillage factor(s).

[b] Knisel, W.G. (Ed.). CREAMS: A Field-Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. USDA, Conservation Research Report No. 26, 1980.

Table 5-13. REDUCTION IN RUNOFF CURVE NUMBERS CAUSED BY CONSERVATION TILLAGE AND RESIDUE MANAGEMENT[a]

Large Residue Crop[b] (lb/acre)	Medium Residue Crop[c] (lb/acre)	Surface Covered by Residue (%)	Reduction in Curve Number[d] (%)
0	0	0	0
400	150	10	0
700	300	19	2
1,100	450	28	4
1,500	700	37	6
2,000	950	46	8
2,500	1,200	55	10
6,200	3,500	90	10

[a] Knisel, W.G. (Ed.). CREAMS: A Field-Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. USDA, Conservation Research Report No. 26, 1980.

[b] Large-residue crop (corn).

[c] Medium residue crop (wheat, oats, barley, rye, sorghum, soybeans).

[d] Percent reduction in curve numbers can be interpolated linearly. Only apply 0 to 1/2 of these percent reductions to CNs for contouring and terracing practices when they are used in conjunction with conservation tillage.

Table 5-14. VALUES FOR ESTIMATING WFMAX IN EXPONENTIAL FOLIAR MODEL

Crop	Yield[a] (Bu/Ac)	Bushel[a] dry wt. (lbs/Bu)	Straw/Grain Ratio	Units Conversion Factor	WFMAX
Corn	110	56	1.0	$1.1214 * 10^{-4}$	1.38
Sorghum	62	56	1.0	$1.1214 * 10^{-4}$	0.78
Soybeans	35	60	1.5	$1.1214 * 10^{-4}$	0.59
Winter wheat	40	60	1.7	$1.1214 * 10^{-4}$	0.72

[a] 10-year average

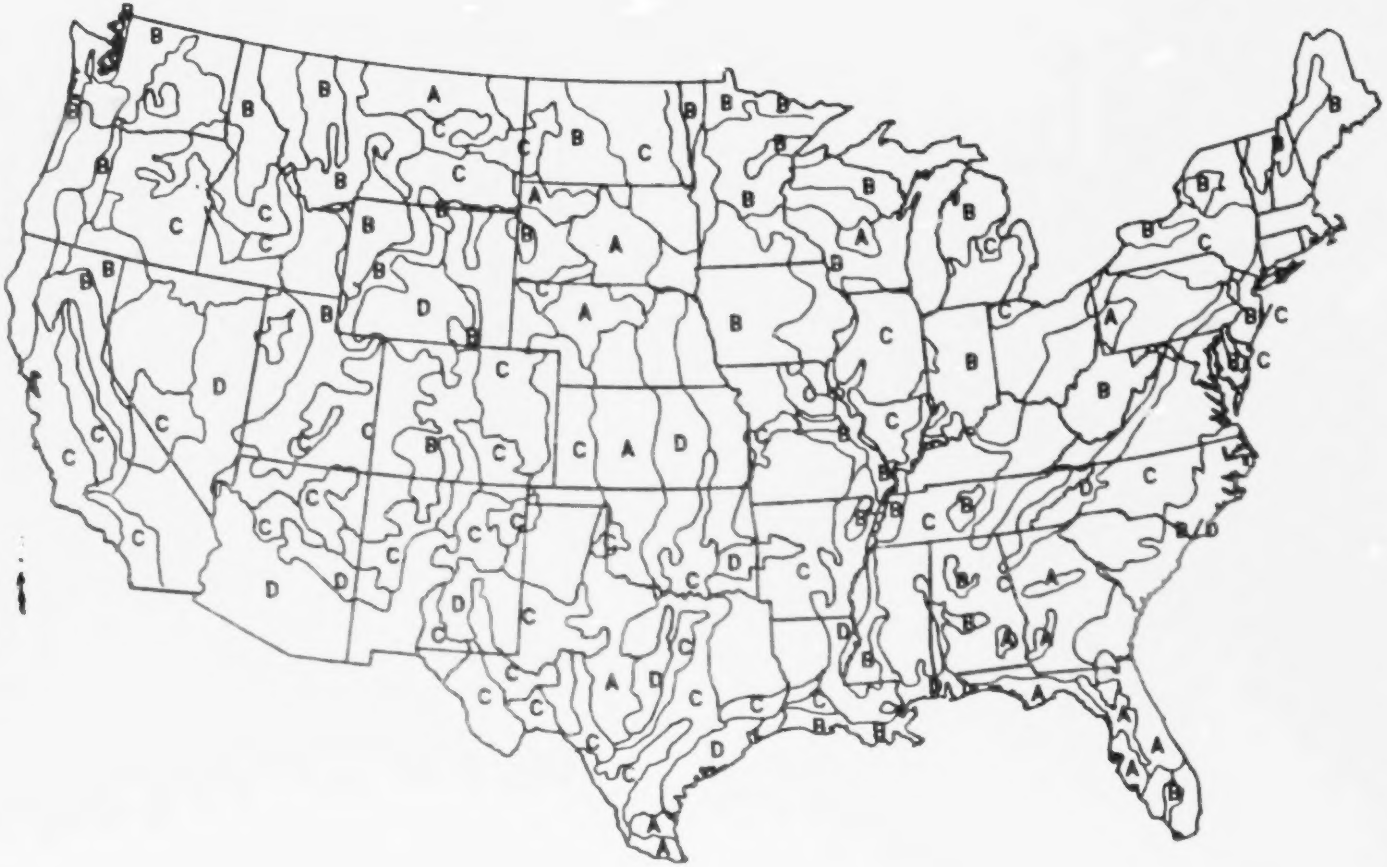

Figure 5.4. Diagram for estimating Soil Conservation Service soil hydrologic groups. (From EPA Field Guide for Scientific Support Activities Associated with Superfund Emergency Response. U.S. Environmental Protection Agency, Corvallis OR, EPA-600/8-82-025.)

Step 2. From Table 5-10 find the land use and treatment or practice that is to be simulated (e.g., row crops, straight row).

Step 3. From Table 5-10 find the hydrologic condition of the soil that is to be simulated (e.g., good).

Step 4. From Table 5-10 find the curve number for antecedent moisture condition II for the site selected. Example: Hydrologic group = A, treatment practice is straight row, land use is row crops, hydrologic condition is good. The curve number for the cropping season is 67.

Step 5. Follow the same procedure for the fallow portion of the growing season using only the hydrologic soil group. Example: Hydrologic soil group A, land use fallow, curve number for condition II is 77.

Step 6. The post-harvest or residue portions of the year requires numbers that reflect the extent of surface cover after harvest. This can be quite variable and in many, cases may require considerable judgement. Under "average" conditions a value set to the mean of the fallow and growing period numbers (from steps 4, 5) is appropriate. In the example case, this number will be the mean of 77 and 67, or 72.

Step 7. The curve number input sequence is now written as

77 67 72

Additional guidance for management practices

Pesticides are being increasingly used in conjunction with conservation practices to reduce erosion and runoff. Most notable among these practices is the use of conservation tillage. The idea is to increase the soil surface residue and hence reduce erosion and runoff by increasing infiltration. The curve numbers developed in steps 1-7 assume conventional practices and must be further modified to reflect the changes in management. Both the fall and growing season numbers must be modified. For purposes of this example, assume the corn is produced by using chisel plows rather than the conventional tillage assumed above. The following steps now apply.

Step 8. From Table 5-11 find the straw/grain ratio for corn, which is 1.0.

Step 9. From Table 5-11 find the bushel weight of corn, which is 56.

Step 10. From Table 5-9 find bushel/acre yield of corn, which is 110.

Step 11. Multiply straw/grain ratio * bushel weight * bushel weight/acre = crop residue produced by the crop. For corn, 1.0 * 56 * 110 = 6160.

Step 12. From Table 5-12 find the tillage practice desired for the crop use site (e.g. chisel plow).

Step 13. Multiply the crop residue determined in step 11 by the tillage factor from step 12 to determine residue remaining, i.e, 6160 * 0.65 = 4004.

Step 14. From Table 5-13 find the reduction in curve number for AMC II, crop curve number produced from residue remaining after harvest determined in step 12. For corn at 4000 pounds per acre, a 10% reduction in curve number is produced.

Step 15. Determine the curve number for antecedent moisture condition (AMC) II. From Steps 1 - 5, AMC II was 67. 67 * 0.10 = 6.7, which is rounded to 7.0. The modified curve numbers are 67 - 7 = 60 and 77 - 7 = 70.

Step 16. The post-harvest curve number must also now be reduced by averaging the fallow and growing season numbers, that is, 70 and 60 to yield 65.

5.2.2 Crop Parameters

COVMAX--Maximum Areal Crop Coverage--
PRZM estimates the ground cover as the crop grows to some maximum value, COVMAX, by linear interpolation between emergence and maturity dates. The maximum areal coverage (COVMAX) determines the fraction of ground covered by the crop and thus influences the mass of pesticide that reaches the ground from an application event. For most crops, the maximum coverage will be on the order of 80 to 100 percent.

WFMAX--Maximum Foliar Dry Weight--
If the user chooses to have the model estimate the distribution between plants and the soil by an exponential function when a pesticide is applied, then WFMAX must be specified. The maximum foliar dry weight, WFMAX, of the plant above ground (kg m^{-2}) is the exponent used in the exponential foliar pesticide application model. Estimates of WFMAX for several major crops were given in Table 5-14. Estimates for other crops will require yield information that is available from the USDA crop reporting service. WFMAX is computed by finding the product of columns 2, 3, and 5, and by multiplying this number by the straw/grain ratio (col. 4) plus 1.0. The straw/grain ratio defines the amount of straw associated with the final grain product. Both the straw and grain should be accounted for to determine the maximum weight. Thus, the straw-to-grain ratio should have 1.0 added to it when used to compute WFMAX. An example is provided for barley.

Step 1. Yield, bushel dry wt., and straw/grain ratio for barley are 42.0, 48.0, and 1.5, respectively.

Step 2. WFMAX = Bu/Ac * Lbs/Bu * (straw/grain ratio + 1.) * conversion factor to yield (kg m^{-2}) for PRZM input.

Step 3. Conversion factor = $2.47 \frac{\text{Ac}}{\text{ha}} * \frac{1 \text{ ha}}{10^4 \text{m}^2} * \frac{0.454 \text{ kg}}{\text{Lbs}} = 1.1214*10^{-4}$

Step 4. WFMAX = $42.0 * 48.0 * (1.5 + 1.0) * 1.1214 \times 10^{-4}$, which equals 0.56.

EMD, EMM, IYREM, MAD, MAM, IYRMAT, HAD, HAM, IYRHAR--Cropping Information for Emergence, Maturity, and Harvest--

Generalized cropping information including date of emergence (EMD, EMM, IYREM), maturity (MAD, MAM, IYRMAT), and harvest (HAD, HAM, IYRHAR) for eight major crops including corn, soybeans, wheat, tobacco, grain sorghum, potatoes, and peanuts were provided in Table 5-9. Simulations involving minor crops such as mint, or where site specific information alters the general practices provided, may require consultation with USDA Handbook No. 283 (Usual Planting and Harvesting Dates) or the local Cooperative Extension Service.

HTMAX--Maximum Canopy Height--

HTMAX is the maximum height of the crop canopy at maturation, and is used in the calculation of the pesticide flux through the plant compartment. Users should have site-specific information for HTMAX since it varies with crop type and species, climate, and environmental conditions. Specific ranges of HTMAX for different crops are listed below:

CROP	HEIGHT (cm)	REF.
Barley	20 - 100	A
Grain Sorghum	90 - 110	B
Alfalfa	10 - 50	A
Corn	80 - 300	A
Potatoes	30 - 60	A
Soybeans	90 - 110	B
Sugarcane	100 - 400	A

References

A. Szeicy et al. (1969)

B. Smith et al. (1978)

5.2.3 Pesticide Parameters

Pesticides can be applied directly to the soil surface, the plant canopy, or to both. Two modeling problems arise when one considers this. First, the initial distribution of the applied pesticide between plant foliage and the soil surface must be estimated. Second, the remaining foliar deposited pesticides then become available for degradation (photolysis) or removal (volatilization, washoff). Recall that two options are available for distributing the applied pesticide (the FAM parameter).

TAPP--Total Pesticide Application--

The total pesticide application per event is entered in terms of kg-active ingredient (a.i.) ha^{-1}. Typical application rates are included on the product's registration label. According to Smith (personal communication, 1988) the coefficient of variation for granular application is 40 to 70% and about 25% for spray application.

DEPI--Depth of Incorporation--
This variable is only needed if soil application of chemical is specified (i.e., FAM = 1). Typical incorporation depths are 5-10 cm. If soil injection is being simulated, user should be aware that injection below 15 to 20 cm is difficult to achieve and represents an approximate upper limit of incorporation depth (Matthews 1979). Representative values for several soil application methods are given in Table 5-15.

Table 5-15. PESTICIDE SOIL APPLICATION METHODS AND DISTRIBUTION

Method of Application	Common Procedure	Distribution	DEPI
Broadcast	Spread as dry granules or spray over the whole surface	Remains on the soil surface	0.0
Disked-in	Disking after broadcast application	Assume uniform distribution to tillage depth (10 cm)	10.0
Chisel-plowed	Chisel plowing after broadcast	Assume linear distribution to tillage depth (15 cm)	15.0
Surface banded	Spread as dry granules or a spray over a fraction of the row	Remains on soil surface	0.0
Banded incorporated	Spread as dry granules or a spray over a fraction of the row and incorporated in planting operation	Assume uniform distribution to depth of incorporation (5 cm)	5.0

FILTRA--Initial Foliage to Soil Distribution--
The filtration parameter (FILTRA) relates to the equation for partitioning the applied pesticide between the foliage and ground (this applies when FAM = 3). Lassey (1982) suggests values in the range of 2.3 -3.3 $m^2 kg^{-1}$. Miller (1979) suggested a value of 2.8 $m^2 kg^{-1}$ for pasture grasses. Most of the variation appears to be due to the vegetation and not the aerosol.

FEXTRC--Foliar Washoff Extraction Coefficient--
Washoff from plant surfaces is modeled using a relationship among rainfall, foliar mass of pesticide, and an extraction coefficient. The parameter (FEXTRC) is the required input parameter to estimate the flux of pesticide washoff. Exact values are varied and depend upon the crop, pesticide properties, and application method. Smith and Carsel (1984) suggest 0.10 is suitable for most pesticides.

IPSCND--Foliage Pesticide Condition Factor--
IPSCND is required only when FAM = 2 or 3. It is a dimensionless number which indicates the disposition of the pesticide remaining on the foliage at and following harvest. IPSEND = 1 indicates that the remaining pesticide on foliage is converted to surface application to the top soil layer; IPSCND = 2 indicates that the remaining foliage pesticide is completely removed with the harvest; and IPSCND = 3 indicates that the remaining foliage pesticide is retained on the surface residue and continues to undergo the same decay and volatilization processes as before.

PLVKRT--Foliage Pesticide First-Order Volatilization Rate--
Pesticide volatilization from plant leaf surfaces is represented as a first-order process controlled by the user-specific rate constant PLVKRT. For organophosphate insecticides, Stamper et al. (1979) have shown that the disappearance rate from leaf surfaces can be estimated by a first-order kinetic approach. Similar observations for first-order kinetics were found for volatilization of 2,4-D iso-octyl ester from leaf surfaces by Grover et al. (1985). Volatilization losses of toxaphene and DDT from cotton plants decreased exponentially with time and were linearly related to the pesticide load on these plants (Willis et al. 1983).

Table 5-16 shows disappearance rates for selected pesticides on plant foliage; these rates are also applicable to estimation of PLVKRT since the overall disappearance rate (PLDKRT) includes loss associated with volatilization. The user must be consistent in specifying these two rates: if PLDKRT includes volatilization processes then PLVKRT should be zero, and if PLVKRT is non-zero then PLDKRT should include all attenuation processes except volatilization. Also, the pesticide volatilization flux controlled by PLVKRT contributes to the calculated pesticide vapor concentration in the atmosphere of the plant canopy, whereas the decay flux controlled by PLDKRT does not.

Recent information (Willis and McDowell 1987) is available for estimating degradation rates of pesticides on plant foliage. In the work cited above, observed half-lives (days) were grouped by chemical family. These were:

- Organochlorine 5.0 ± 4.6
- Organophosphorus 3.0 ± 2.7
- Carbamate 2.4 ± 2.0
- Pyrethroid 5.3 ± 3.6

These mean half-lives correspond to degradation rates of 0.14, 0.23, 0.29 and 0.13 day^{-1}, respectively. These are in reasonable agreement with the values

Table 5-16. DEGRADATION RATE CONSTANTS OF SELECTED PESTICIDES ON FOLIAGE[a]

Class	Group	Decay Rate (days^{-1})
Organochlorine	Fast (aldrin, dieldrin, ethylan, heptachlor, lindane, methoxychlor).	0.2310 - 0.1386
	Slow (chlordane, DDT, endrin, toxaphene).	0.1195 - 0.0510
Organophosphate	Fast (acepate, chlorphyrifos-methyl, cyanophenphos, diazinon, depterex, ethion, fenitrothion, leptophos, malathion, methidathion, methyl parathion, phorate, phosdrin, phosphamidon, quinalphos, alithion, tokuthion, triazophos, trithion).	0.2772 - 0.3013
	Slow (azinphosmethyl, demeton, dimethoate, EPN, phosalone).	0.1925 - 0.0541
Carbamate	Fast (carbofuran)	0.630
	Slow (carbaryl)	0.1260 - 0.0853
Pyrethroid	(permethrin)	0.0196
Pyridine	(pichloram)	0.0866
Benzoic acid	(dicamba)	0.0745

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[a] Knisel, W.G. (Ed.). CREAMS: A Field-Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. USDA, Conservation Research Report No. 26, 1980.

in Table 5-16 with the exception of the pyrethroids, which appear to have a faster breakdown than Table 5-16 suggests.

If the user has monitoring data which shows the degradation of plant foliar concentrations with time, then the coefficient can be calibrated to cause the simulated concentrations to mimic the observed data. The exponential decay model is given by:

$$C = C_o e^{-(FEXTRC)t} \tag{5-1}$$

where

C = simulated concentration

C_o = initial concentration

FEXTRC= first order decay rate (day^{-1})

t = time elapsed since application (days)

In linear form the equation is

$$\ln (C/C_o) = -(FEXTRC)t \tag{5-2}$$

Therefore, the coefficient FEXTRC is the slope of the plot of the natural log of the normalized concentrations (C/C_o) vs. time in days. Obviously, loss rates calculated in this way include volatilization losses and the above caveats apply.

DAIR--Vapor Phase Diffusion Coefficient--
The diffusion coefficient is defined by Fick's first law, as the proportionality between the chemical flux and the spatial gradient in its concentration (Nye 1979) (see Volume I, Section 2.3.4). DAIR for a chemical depends on both its own characteristics and those of the medium through which the chemical is diffusing.

In soil, vapor phase diffusion occurs in the soil air space. Each chemical will in general have its own characteristic diffusion coefficient depending on its molecular weight, molecular volume, and shape (Streile 1984). However, Jury et al. (1983) have concluded that the diffusion coefficient will not show significant variations for different pesticides at a given temperature; they recommend using a constant value of 0.43 m^2 day^{-1} for all pesticides.

Thibodeaux and Scott (1985) calculated values in the range of 0.39 to 0.78 m^2 day^{-1} for 12 benchmark chemicals exhibiting a broad spectrum of characteristics. Included in this list was chlorpyrifos and DDT, with calculated vapor diffusion coefficients of 0.39 and 0.40 m^2 day^{-1}, respectively. Consequently, we concur with Jury's recommendation to use 0.43

m^2 day^{-1} for all pesticides, unless other chemical-specific data are available to justify a different value. Note that the DAIR parameter is entered in cm^2 day^{-1}. The user should take care to convert the above recommended values.

Although the magnitude of DAIR will likely increase with soil temperature, very little information is available to quantify this dependence. Accordingly, no temperature adjustment for DAIR is performed in the volatilization model.

HENRYK--Henry's Constant--
Henry's constant is a ratio of a chemical's vapor pressure to its solubility. It represents the equilibrium between the vapor and solution phases, and can be calculated as follows:

$$H = P/S \tag{5-3}$$

where

H = Henry's constant (atm-m^3 $mole^{-1}$)

P = partial pressure of pesticide (atm)

S = aqueous solubility of pesticide (mole m^{-3})

It is quite common in environmental modeling applications to express Henry's constant on a dimensionless basis, which implies a variant form of relationship, as follows:

$$K_H = \frac{C_V}{C_L} \tag{5-4}$$

where

K_H = dimensionless Henry's constant

C_V = saturated vapor density of pesticide (mg l^{-1})

C_L = aqueous solubility of pesticide (mg l^{-1})

Henry's constant can be converted from atm-m^3 $mole^{-1}$ to a dimensionless number by multiplying by 44.64 (Schnoor et al. 1987). Specific values of HENRYK for selected pesticides can be found in Table 5-17. Many of these values are calculated from Equation (2) by estimating the saturated vapor density and aqueous solubility of the pesticide. Both Jury et al. (1984) and Schnoor et al. (1987) have tabulated values of HENRYK for other chemicals.

Table 5-17. ESTIMATED VALUES OF HENRY'S CONSTANT FOR SELECTED PESTICIDES

Compound	Henry's Constant (dimensionless)	References
Alachlor	1.3E-06	A
Aldrin	6.3E-04	D
Anthracene	4.4E-05	D
Atrazine	2.5E-07	A
Bentazon	2.0E-10	A
Bromacil	3.7E-08	C
Butylate	3.3E-03	A
Carbaryl	1.1E-05	A
Carbofuran	1.4E-07	A
Chlorpyrifos	1.2E-03	A
Chrysene	4.7E-05	D
Cyanazine	1.2E-10	A
DDT	2.0E-03	C
Diazinon	5.0E-05	C
Dicamba	3.3E-08	A
Dieldrin	6.7E-04	C
Diuron	5.4E-08	C
Endrin	1.8E-05	D
EPTC	5.9E-04	C
Ethoprophos	6.0E-06	C
Fenitrothion	6.0E-06	B
Fonofos	2.1E-04	A
Heptachlor	1.7E-02	D
Lindane	1.3E-04	B
Linuron	2.7E-06	A
Malathion	2.4E-06	B
Methomyl	4.3E-08	A
Methyl Parathion	4.4E-06	A
Metolachlor	3.8E-07	A
Metribuzin	9.8E-08	A
Monuron	7.6E-09	C
Napropamide	7.9E-07	C
Parathion	6.1E-06	C
Permethrin	6.2E-05	A
Picloram	1.9E-08	B
Prometryne	5.6E-07	C
Simazine	1.3E-08	A
Terbufos	1.1E-03	A
Toxaphene	2.3E+00	A
Triallate	7.9E-04	C
Trichlorfon	1.5E-09	B
Trifluralin	6.7E-03	A
2,4-D (acid)	5.6E-09	A
2,4,5-T (acid)	7.2E-09	B

References: A - Donigian et al. (1986); B - Spencer et al. (1984)
C - Jury et al. (1984); D - Schnoor et al. (1987)

ENPY--Enthalpy of Vaporization--
This parameter is used in the temperature correction equation for Henry's constant (as described in Volume I, Section 2.3.4). In our limited literature search, we could find only two pesticides with ENPY values reported: 18.488 Kcal $mole^{-1}$ for lindane and 20.640 Kcal $mole^{-1}$ for napropamide (Streile 1984). Chemical-specific values are needed for ENPY, however, it appears that a value of 20 Kcal $mole^{-1}$ is a reasonable first guess.

KD--Pesticide Soil-Water Distribution Coefficient--
The user can enter directly the distribution coefficient(s) or the model will calculate a value given other pesticide properties. If the parameter KDFLAG is set to a value of 0, then direct data input is made as the parameter KD. If KDFLAG is set to 1, however, the following additional information is required.

PCMC, SOL--Options for Use in Estimating Distribution Coefficients from Related Input Data--
The fate of pesticides in soil and water is highly dependent on the sorptive characteristics of the compound. Sorptive characteristics affect the physical movement of pesticides significantly. The sorptive properties of pesticides generally correlate well with the organic carbon content of soils. The carbon content of most soils decreases with depth.

PRZM allows the user to estimate an organic carbon partition coefficient for the pesticide from one of three models based on water solubility. The K_{oc} is subsequently multiplied by organic carbon to obtain the partition coefficient. The three models are:

PCMC1 $$\text{Log } K_{oc} = (-0.54 * \text{Log SOL}) + 0.44 \qquad (5\text{-}5)$$

K_{oc} = organic carbon distribution coefficient

where SOL = water solubility, mole fraction

PCMC2 $$\text{Log } K_{oc} = 3.64 - (0.55 * \text{Log SOL}) \qquad (5\text{-}6)$$

where SOL = water solubility, mg l^{-1}

PCMC3 $$\text{Log } K_{oc} = 4.40 - (0.557 * \text{Log SOL}) \qquad (5\text{-}7)$$

where SOL = water solubility, micromoles l^{-1}

These models are selected by setting PCMC to values of 1, 2, or 3, respectively. These methods were selected because of referenced documentation and provisions for direct use with the most commonly reported physical pesticide parameter, water solubility. The three models used in PRZM for estimating partitioning between soil and water are limited to specific types of pesticides. These equations are best used for pesticides having melting points below 120 °C. Solubilities above these temperatures are affected by crystalline energy and other such physical properties. The three models are not appropriate for pesticides whose solubilities are affected by crystalline energy or other physical properties, and would have a tendency to overestimate the partitioning between soil and water. Of the three models, the first model is for true equilibrium of completely dispersed particles of soil/water concentrations less than 10.0 g l^{-1}. The second and third models are for soil/water concentrations greater than 10.0 g l^{-1} and for short equilibrium periods of 48 hours or less. For most applications, the first model would be the most appropriate.

Some pesticides having properties amenable for use with the water solubility models are provided in Table 5-18. The pesticide solubility, SOL, must also be input. Units must be consistent with the model chosen. Table 5-18 also provides pertinent values for the selected pesticides.

Alternative methods are available to calculate K_{oc}. A useful relationship exists between the octanol-water distribution coefficient and the organic carbon distribution coefficient. This relationship can be used when measured soil distribution coefficients are not available, or the pesticides posses crystalline energy properties that would preclude the use of any water solubility models.

The octanol-water distribution coefficient can be used for calculating distribution coefficients for pesticides that possess monomer-associated properties for solubility in water. Karickhoff et al. (1979) proposed a relationship between K_{ow} and K_{oc} given by

$$\log K_{oc} = 1.00 (\log K_{ow}) - 0.21 \qquad (5\text{-}8)$$

where

K_{ow} = octanol-water distribution coefficient (cm^3 g^{-1})

K_{oc} = organic carbon distribution coefficient (cm^3 g^{-1})

Carbofuran is a pesticide that exhibits crystalline energy relationships and its apparent distribution coefficient should be estimated using its log K_{ow}, which is 2.44. Substituting into equation (5-8)

$$\log K_{oc} = 1.00 (2.44) - 0.21 = 2.23$$

$$K_{oc} = 10^{2.23} = 169.8$$

For a soil with 0.5% organic carbon the K_d of the pesticide is

$$K_d = K_{oc} \frac{\text{(percent organic carbon)}}{100} \qquad (5\text{-}9)$$

$$K_d = \frac{169.8\ (0.5)}{100} = 0.85$$

Table 5-18. PHYSICAL CHARACTERISTICS OF SELECTED PESTICIDES FOR USE IN DEVELOPMENT OF PARTITION COEFFICIENTS (USING WATER SOLUBILITY) AND REPORTED DEGRADATION RATE CONSTANTS IN SOIL ROOT ZONE

Chemical	Common Name	Solubility in Water (Temp. 20-25°C) (mg/l)	Mode of Action						Molecular weight (g)	Reference	Partitioning Model			Degradation Rate Constant in Soil Root Zone (days^{-1})	Reference
			Reference	Insecticide	Herbicide	Fungicide	Nematocide	Acaricide			PCMC1 (mole fraction)	PMCM2 (mg/l)	PCMC3 (um/l)		
Actellic	pirimiphosmethyl	5	a	X					274	b	$3.28*10^{-7}$	5	18		
Alachlor	alachlor	220	b		X				269.9	b	$1.47*10^{-5}$	220	815	.0384	f
Antor	diethatyl ethyl	105	a		X				311.5	c	$6.07*10^{-6}$	105	337	.0099-.0173	g
Aresin	monolinuron	735	a		X				214.6	b	$6.17*10^{-5}$	735	3430		
Balan	benefin	70	b		X				335.3	b	$3.76*10^{-6}$	70	209	0.3349	f
Basalin	fluchloralin	0.7	b		X				355.7	b	$3.55*10^{-8}$	0.7	2	0.0169	f
Baygon	propoxur	2000	a	X					209	b	$1.72*10^{-4}$	2000	9600		
Baygon Meb	plifenate	50	a	X					336.2	d	$2.68*10^{-6}$	50	149		
Bayleton	triadimefon	70	a			X			267.45	d	$4.72*10^{-6}$	70	262		
Baythion	phoxim	7	b	X					298	b	$4.23*10^{-7}$	7	24		
Baythion C	chlorphoxim	1.7	a	X					301.45	d	$1.02*10^{-7}$	1.7	5.6		
Betasan	bensulide	25	c		X				397.5	b	$1.13*10^{-6}$	25	63		
Bromophos	bromophos	40	a	X					366	b	$1.97*10^{-6}$	40	109	.0198	f
Butachlor	butachlor	23	a		X				312	e	$1.33*10^{-6}$	23	74		
Bux	bufencarb	1	b	X					221.3	b	$8.14*10^{-8}$	1.0	5		
Carbamult	promecarb	92	a	X					207	d	$8.01*10^{-6}$	92	444		
Carbyne	barban	11	c		X				258.1	b	$7.70*10^{-7}$	11	43	.0347	g
Chlordimeform	chlordimeform	250	a	X				X	196.7	b	$2.30*10^{-5}$	250	1270		
Chlorfenvinphos	chlorfenvinphos	110	a	X					359.5	b	$5.51*10^{-6}$	110	306	.0055	f
Chloro IPC	chlorpropham	108	b		X				213.7	b	$9.11*10^{-6}$	108	505	.0058-.00267	g
Chlorpyrifos	chlorpyrifos	2	b	X					350.5	b	$1.03*10^{-7}$	2.0	6		
Co-Ral	coumaphos	1.5	b	X					362.8	b	$7.45*10^{-8}$	1.5	4		
Counter	terbufos	15	a	X			X		288	d	$9.38*10^{-7}$	15	52		
DNOC	DNOC	130	a	X	X	X			198.1	b	$1.18*10^{-5}$	130	656		
Dichlorprop	dichlorprop	350	a		X				235	b	$2.68*10^{-5}$	350	1490	.0578-.0866	f
Dimetan	dimetan	30000	b	X					197.3	b	$2.74*10^{-3}$	30000	152000		
Dimethoate	dimethoate	$\bar{X}$=25000	a	X					229.1	b	$1.97*10^{-3}$	25000	109000	.0057	
Dinitramine	dinitroamine	1	a		X				322.2	c	$5.60*10^{-8}$	1	3	.0193-.0856	f
Dinoseb	dinoseb	52	c		X				240.2	b	$3.90*10^{-6}$	52	217	.0462-.0231	g
Dazomet	dazomet	1200	b		X	X	X		162.3	b	$1.33*10^{-4}$	1200	7390		
Devrinol	napropamide	73	a		X				271.36		$4.85*10^{-6}$	73	269		
Elocron	dioxacarb	6000	a	X					223	b	$4.85*10^{-4}$	6000	26900	.3465-.0248	f
Evik	ametryn	185	a		X				227	b	$1.47*10^{-5}$	185	815	.0231-.0077	g
Far-Go	triallate	4	b		X				304.6	b	$2.37*10^{-7}$	4	13	.0231-.0713	g
Fongarid	furalaxyl	230	a			X			301	d	$1.38*10^{-5}$	230	764		

Table 5-18. PHYSICAL CHARACTERISTICS OF SELECTED PESTICIDES FOR USE IN DEVELOPMENT OF PARTITION COEFFICIENTS (USING WATER SOLUBILITY) AND REPORTED DEGRADATION RATE CONSTANTS IN SOIL ROOT ZONE (CONTINUED)

Chemical	Common Name	Solubility in Water (Temp. 20-25°C) (mg/l)	Reference	Mode of Action: Insecticide	Herbicide	Fungicide	Nematocide	Acaricide	Molecular weight (g)	Reference	Partitioning Model: PCMC1 (mole fraction)	PMCM2 (mg/l)	PCMC3 (um/l)	Degradation Rate Constant in Soil Root Zone (days^{-1})	Reference
Fornothion	fornothion	2600	a	X				X	257	b	$1.82*10^{-4}$	2600	10100		
Fuji-one	isoprothiolane	48	a	X		X			290	d	$2.98*10^{-6}$	48	166		
Gardona	tetrachlorvinphos	11	b	X					366	b	$5.42*10^{-7}$	11	30	.1732-.1386	
Gesaran	methoprotryne	320	a		X				271	b	$2.13*10^{-5}$	320	1180		
Goal	oxyfluorfen	0.1	c		X				361.7	c	$4.98*10^{-9}$	0.1	0.3	.0231-.0173	c
Guthion	azinphos-methyl	29	a	X					317.3	b	$1.65*10^{-6}$	29	91	.0533-.0014	f
Hoelon	diclofop methyl	30	a		X				340.9	d	$1.59*10^{-6}$	30	88		
Imidan	phosmet	25	b	X					317.3	b	$1.42*10^{-6}$	25	79		
IPC	propham	250	b		X				179.2	b	$2.51*10^{-5}$	250	1400	.0347-.0116	g
Linuron	linuron	75	a		X				249.1	b	$5.42*10^{-6}$	75	300	.0280-.0039	f
Malathion	malathion	145	a	X					330.4	b	$7.91*10^{-6}$	145	439	2.91-.4152	f
Mecoprop	mecoprop	620	a		X				214.6	b	$5.21*10^{-5}$	620	2890		
MEMC	MEMC	50000	a			X			295	d	$3.05*10^{-3}$	50000	169000		
Merpelan AZ	isocarbamid	13000	a		X				185	d	$1.27*10^{-3}$	13000	70300		
Mesoranil	aziprotryn	75	b		X				225	b	$6.01*10^{-6}$	75	333		
Mesurol	mercaptodimethur	$2.7*10^{7}$	a	X					225.3	b	2.16	$2.7*10^{7}$	$1.2*10^{8}$		
Methomyl	methomyl	58000	a	X					162.2	b	$6.44*10^{-3}$	58000	358000		
Methoxychlor	methoxychlor	0.1	b	X					345.7	b	$5.21*10^{-9}$	0.1	0.3	.0046-.0033	f
Meth-Parathion	methyl Parathion	$\bar{X}$=57.5	a	X					263.2	b		57.5	219	.2207	f
Nemacur	fenamiphos	400	a			X			303	b	$2.38*10^{-5}$	400	1320		
Nortron	ethofumesate	110	a		X				286	d	$6.93*10^{-6}$	110	385		
Orthene	acephate	$6.5*10^{5}$	b	X					183.2	b	0.06	650000	3550000		
Oxamyl	oxamyl	$2.8*10^{5}$	a	X			X	X	219	b	0.023	280000	1280000	.0354-.0646	f
Parathion	parathion	24	b	X					291.3	b	$1.48*10^{-6}$	24	82	.2962-.0046	f
Patoran	metabromuron	330	a		X				258.9	d	$2.30*10^{-5}$	330	1280	.0234	f
Phorate	phorate	50	b	X					260.4	b	$3.46*10^{-6}$	50	192	.0363-.0040	f
Propachlor	propachlor	580	c		X				211.7	b	$4.94*10^{-5}$	580	2740	.0231-.0139	g
Propanil	propanil	500	c		X				218	b	$4.13*10^{-5}$	500	2290	.693-.231	g
Prowl	pendimethalin	0.5	c		X				281.3	c	$3.20*10^{-8}$	0.5	1.8		
Prynachlor	prynachlor	500	a		X				221.7	b	$4.06*10^{-5}$	500	2260		
Quinalphos	quinalphos	22	a	X				X	298	d	$1.33*10^{-6}$	22	74		
Ronstar	oxadiazon	0.7	b		X				345.23	b	$3.65*10^{-8}$	0.7	2.0		
Sancap	dipropetryn	16	a		X				255.4	b	$1.13*10^{-6}$	16	63		

Table 5-18. PHYSICAL CHARACTERISTICS OF SELECTED PESTICIDES FOR USE IN DEVELOPMENT OF PARTITION COEFFICIENTS (USING WATER SOLUBILITY) AND REPORTED DEGRADATION RATE CONSTANTS IN SOIL ROOT ZONE (CONCLUDED)

				Mode of Action							Partitioning Model				
Chemical	Common Name	Solubility in Water (Temp. 20-25°C) (mg/l)	Reference	Insecticide	Herbicide	Fungicide	Nematocide	Acaricide	Molecular weight (g)	Reference	PCMC1 (mole fraction)	PMCM2 (mg/l)	PCMC3 (um/l)	Degradation Rate Constant in Soil Root Zone (days^{-1})	Reference
Semeron	desmetryn	580	a		X				213	b	$4.91*10^{-5}$	580	2720		
Supracide	methidathion	240	a	X				X	302	b	$1.43*10^{-5}$	240	795	.0495-.0108	f
Tachigareu	hymexazol	85000	a			X			99.05	b	0.02	85000	858000		
Temik	aldicarb	6000	a	X			X	X	190.3	b	$5.68*10^{-4}$	6000	31500	.0322-.0116	f
Tolban	profluralin	0.1	a		X				347.3	c	$5.19*10^{-9}$	0.1	0.3	.0049	f
Trifluralin	trifluralin	24	b		X				335.3	b	$1.29*10^{-6}$	24	71	.0956-.0026	f
Tsumacide	MTMC	2600	a	X					165	d	$2.84*10^{-4}$	2600	15800		
Tordon	picloram	430	c		X				241.5	b	$3.21*10^{-5}$	430	1780	.0354-.0019	f
Toxaphene	toxaphene	3	b	X					413	b	$1.31*10^{-7}$	3	7	.0046	f
Trichlorfon	trichlorfon	120000	a	X					257.35	d	$8.40*10^{-3}$	120000	466000		

Calculations for the Karickhoff and Chiou partitioning equations are:

PCMC1: $\frac{\text{ppm solubility}}{\text{molecular weight (g)}}$ = millimole solubility (MMS); $\frac{MMS}{10^3}$ = molar solubility (MS); $\frac{MS}{55.5 \text{ (molar conc. water)}}$ = mole fraction

Chiou: $\frac{\text{ppm solubility}}{\text{molecular weight (g)}}$ = millimole solubility (MMS); $\frac{MMS}{10^3} * 10^6$ = um/l

References

[a] Farm Chemical Handbook, Meister Publishing Company, Willoughby, OH (1981).

[b] Pesticide Manual, issued by the British Crop Protection Council, 1968.

[c] Herbicide Handbook of the Weed Science Society of America, 4th ed. 1979.

[d] Calculations based on information from Farm Chemical Handbook, 1981.

[e] Analytical Reference Standards and Supplemental Data for Pesticides and Other Organic Compounds, U.S. EPA-600/2-81-011, 1981.

[f] Nash, R.G. 1980. Dissipation Rate of Pesticides from Soils. Chapter 17. IN CREAMS: A Field Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. W.G. Knisel, ed. USDA Conservation Research Report No. 26. 643 pp.

[g] Control of Water Pollution from Cropland, Vol. I, a manual for guideline development, EPA-600/2-75-026a.1

This compares to an estimated K_d of 2.68 using the PCMCl water solubility model and the same organic carbon content. Selected pesticides having properties suitable use with the octanol water distribution model by Karickhoff are provided in Table 5-19.

DWRATE, DSRATE--Degradation Rate Constants--
The processes that contribute to pesticide disappearance in soils are varied and depend on environmental factors as well as chemical properties. Unfortunately, only rarely are process-specific rate constants (e.g., hydrolysis) reported for the soil environment. In most cases, a lumped first-order rate constant is assumed. This is the model used in PRZM, with the additional enhancement of allowing the user to specify different decay rates for the solution (DWRATE) and sorbed (DSRATE) phases. Although such an approximation is imprecise, most modeling efforts follow a similar approach and many pesticides appear to behave in this manner. For example, Nash (1980) found that disappearance of many compounds was highly correlated to a first order approximation with $R^2 \geq 0.80$. More recently, Rao et al. (1984) reported that pesticide disappearance rate constants in surface horizons of soils (root zone) are reasonably constant across soils. This is encouraging from a modeling standpoint because of the decrease in sensitivity testing required for dissipation rates.

The dissipation rate of pesticides below the root zone, however, is virtually unknown. Several studies have suggested the rate of dissipation decreases with depth; however, no uniform correction factor was suggested between surface/subsurface rates. First order dissipation rates for selected pesticides in the root zone were tabulated in Tables 5-18 and 5-19.

For most cases, the same values should be used for both DWRATE and DSRATE, and for all depths, unless specific investigations indicate otherwise. For example, Macalady and Wolfe (1984) have concluded that the relative abiotic hydrolysis rates for the solution and sorbed phases for several pesticides depend on the specific hydrolytic pathway. For neutral hydrolysis, the rates are similar in both phases; whereas for alkaline hydrolysis the sorbed phase rate is retarded (i.e., less than), and for acid hydrolysis it is accelerated (i.e., greater than) compared to the solution phase rate. Although it is not currently possible to predict the magnitude of the change for all pesticides (Wolfe 1988), specific laboratory studies for organophosphate insecticides showed a decrease in alkaline hydrolysis rates by a factor of 10 for the sorbed phase compared to the solution phase (Macalady and Wolfe 1985).

With regard to changes in the decay rate with depth, studies by Lavy et al. (1973) and Wehtje et al. (1984) for atrazine showed a 0.5 and 0.3 reduction, respectively, between surface and subsurface attenuation rates; work by Smelt et al. (1978) on aldicarb showed similar reductions. Studies of this type, and those noted above on hydrolysis rates, can be used to justify different decay rates for DWRATE and DSRATE, and for different soil depths, if the experimental conditions are similar or consistent with the site being simulated.

Table 5-19. OCTANOL WATER DISTRIBUTION COEFFICIENTS (log K_{ow}) AND SOIL DEGRADATION RATE CONSTANTS FOR SELECTED CHEMICALS

Chemical Name	Log K_{ow}[b]	Degradation Rate Constant (days^{-1})	Reference
Alachlor	2.78	0.0384	A
Aldicarb	0.70	0.0322 - 0.0116	A
Altosid	2.25		
Atrazine	2.45	0.0149 - 0.0063	A
Benomyl	2.42	0.1486 - 0.0023	A
Bifenox	2.24	0.1420	A
Bromacil	2.02		
Captan	2.35		
Carbaryl	2.56	0.1196 - 0.0768	A
Carbofuran	2.44	0.0768 - 0.0079	A
Chloramben	1.11		
Chlordane	4.47	0.0020 - 0.0007	
Chloroacetic Acid	-0.39		
Chloropropham	3.06	0.0058 - 0.00267	D
Chloropyrifos	4.97		
Cyanazine	2.24	0.0495	C
Dalapon	0.76	0.0462 - 0.0231	D
Dialifor	4.69		
Diazinon	3.02	0.0330 - 0.0067	A
Dicamba	0.48	0.2140 - 0.0197	A
Dichlobenil	2.90	0.0116 - 0.0039	
Dichlorofenthion	5.14		
2,4,-Dichlorophenoxy-acetic Acid	2.81	0.0693 - 0.0231	D
Dichloropropene	1.73		
Dicofol	3.54		
Dinoseb	2.30	0.0462 - 0.0231	D
Diuron	2.81	0.0035 - 0.0014	D
Endrin	3.21		
Fenitrothion	3.36	0.1155 - 0.0578	A
Fluometuron	1.34	0.0231	C
Linuron	2.19	0.0280 - 0.0039	A
Malathion	2.89	02.91 - 0.4152	A
Methomyl	0.69		
Methoxychlor	5.08	0.0046 - 0.0033	A
Methyl Parathion	3.32	0.2207	A
Monolinuron	1.60		
Monuron	2.12	0.0046 - 0.0020	D
MSMA	-3.10		
Nitrofen	3.10		
Parathion	3.81	0.2961 - 0.0046	A
Permethrin	2.88	0.0396	E
Phorate	2.92	0.0363 - 0.0040	A

Table 5-19. OCTANOL WATER DISTRIBUTION COEFFICIENTS (log K_{ow}) AND SOIL DEGRADATION RATE CONSTANTS FOR SELECTED CHEMICALS (concluded)

Chemical Name	Log K_{ow}[b]	Degradation Rate Constant (days^{-1})	Reference
Phosalone	4.30		
Phosmet	2.83		
Picloram	0.30	0.0354 - 0.0019	A
Propachlor	1.61	0.0231 - 0.0139	D
Propanil	2.03	0.693 - 0.231	D
Propazine	2.94	0.0035 - 0.0017	D
Propoxur	1.45		
Ronnel	4.88		
Simazine	1.94	0.0539 - 0074	A
Terbacil	1.89		
Terbufos	2.22		
Toxaphene	3.27	0.0046	E
Trifluralin	4.75	0.0956 - 0.0026	A
Zineb	1.78	0.0512	A

[A] Nash, R. G. 1980. Dissipation Rate of Pesticides from Soils. Chapter 17. IN CREAMS: A Field Scale Model for Chemicals, Runoff, and Erosion from Agricultural Management Systems. W. G. Knisel, ed. USDA Conservation Research Report No. 26. 643pp.

[B] Smith, C. N. Partition Coefficients (Log K_{ow}) for Selected Chemicals. Athens Environmental Research Laboratory, Athens, GA. Unpublished report, 1981.

[C] Herbicide Handbook of the Weed Science Society of America, 4th ed. 1979.

[D] Control of Water Pollution from Cropland, Vol. I, a manual for guideline development, EPA-600/2-75-026a.

[E] Smith, C. N. and R. F. Carsel. Foliar Washoff of Pesticides (FWOP) Model: Development and Evaluation. Accepted for publishing in Journal of Environmental Science and Health - Part B. Pesticides, Food Contaminants, and Agricultural Wastes, B 19(3), 1984.

DGRATE--First Order Decay Rate for Vapor-Phase Pesticide--
Pesticide degradation in soils is a kinetic phenomenon. Pesticides are degraded by different mechanisms, and at different rates, depending upon whether they are in vapor, liquid or adsorbed phase (Streile 1984). A lumped first-order rate constant is assumed for DGRATE. In general, a zero value of DGRATE is recommended, unless chemical-specific data is available to justify a non-zero value. For example, if the user is calibrating for a highly volatile and/or photo-sensitive chemical, vapor phase attenuation processes in the upper 1-2 mm of the soil surface may be very important. Field studies have shown that photo chemical loss of organic chemicals may be rapid and substantial immediately following application to the land surface, especially in the case of hydrophobic or cationic organics that sorb to soil particles (Miller et al. 1987).

UPTKF--Plant Uptake of Pesticides--
The plant uptake efficiency factor, or root reflection coefficient (UPTKF) provides for removal of pesticides by plants and is a function of the crop root distribution and the interaction of soil, water, and the pesticide. Several approaches to modeling the uptake of nutrients/ pesticides have been proposed ranging from process models that treat the root system as a distribution sink of known density or strength to empirical approaches that assume a relationship to the transpiration rate. Dejonckheere et al. (1983) reported the mass of uptake into sugar beets for the pesticides aldicarb and thiofanox for three soils (sandy loam, silt loam, and sandy clay loam). Mass removal expressed as a percentage of applied material for aldicarb on sandy loam, silt loam, and clay loam ranged from 0.46-7.14%, 0.68-2.32%, and 0.15-0.74%, respectively. For thiofanox, 2.78-20.22%, 0.81-8.70%, and 0.24-2.42% removals were reported for the respective soils. The amount of uptake was higher for sandy soils and increased with available water. Other reviews have suggested ranges from 4-20% for removal by plants.

The procedure adopted for PRZM estimates the removal of pesticides by plant uptake based on the assumption that uptake of the pesticide is directly related to the transpiration rate. Sensitivity tests conducted with PRZM indicate an increase in the uptake by plants as the root zone depth increases, and as the partition coefficient decreases. For highly soluble pesticides and for crop root zones less than 120 cm, the model simulates total uptake within the range reported by Dejonckheere, et al. For highly soluble pesticides and for crop root zones of greater than 120 cm, values of greater than 20% were simulated. For initial estimates a value of 1.0 for UPTKF is recommended. If more than 20-25% of the pesticide is simulated (to be removed by plant uptake), UPTKF should be calibrated to a value less than 1.0.

CORED--Thickness of Soil Column--
The user will want to enter a typical value for the crop root zone unless PRZM is not used in conjunction with VADOFT. For use with SAFTMOD, the PRZM core depth would be extended to the bottom of the first aquifer.

DISP--Dispersion--
The dispersion or "smearing out" of the pesticide as it moves down in the soil profile is attributed to a combination of molecular diffusion and

hydrodynamic dispersion. The transport equations solved in PRZM also produce truncation error leading to a purely mathematical or numerical dispersion. The terms dropped from the Taylor's series expansion from which the finite difference equations were formulated lead to errors that appear identical to the intentional expressions for hydrodynamic dispersion. For these reasons the DISP parameter must be evaluated in light of both "real" and "numerical" components.

Molecular diffusion, D_m, in soils will be lower than free-water diffusion and has been estimated by Bresler (1973)

$$D_m = D_w \, a e^{b\theta} \tag{5-10}$$

where

D_w= molecular diffusion in free water, $cm^2 \, day^{-1}$

a= soil constants having a range of 0.001 to 0.005

b= soil constant having an approximate value of 10

θ= volumetric water content, $cm^3 \, cm^{-3}$

The free-water diffusion coefficient, D_w, can be estimated from procedures outlined by Lyman et al. (1982). In any case, values are quite low, typically less than 10^{-6} $cm^2 \, day^{-1}$, and can usually be ignored.

Hydrodynamic dispersion is more difficult to estimate because of its site-soil specificity and its apparent strong dependence upon water velocity. Most investigators have established an effective diffusion or dispersion coefficient that combines both molecular and hydrodynamic terms. This combined expression can then be related to system variables by developing expressions from field measurements. Most notable among these expressions is

$$D = 0.6 + 2.93 \, v^{1.11} \tag{5-11}$$

where

D= effective dispersion coefficient, $cm^2 \, day^{-1}$

v= pore water velocity, $cm \, day^{-1}$

by Biggar and Nielsen (1976). Note in Equation (5-11) D is a time-and depth-varying function since v is both time and depth-varying. The problem remains to estimate the assumed constant value for DISP, the effective dispersion coefficient.

As previously noted, the backward difference numerical scheme in the PRZM code for solution of the transport equation produces numerical dispersion. This dispersion is also related to the magnitude of the velocity term. Other variables that influence the truncation error include the time and space steps. Because this dispersion is a function of velocity, it is not possible to illustrate the entire range for all anticipated modeling problems. A sensitivity analysis was performed, however, to examine the influence of the spatial step, Δx. Results are given in Figure 5.5. For these runs the DISP parameter was set to 0.0.

The influence of the DISP parameter superimposed on the numerical dispersion created by the model at a Δx value of 5.0 cm is shown in Figure 5.6. Clearly, even when moderate values for DISP are used, substantial dispersion is produced. If equation 5-11 is used along with typical simulated values for velocity (0.1 - 22 cm day^{-1}), then calculated DISP values range from 0.83 - 91 cm^2 day^{-1}. It is clear that if this procedure is used, the desired dispersion will be substantially higher than it should be because of the model's numerical dispersion.

A number of modeling studies were performed to investigate the impact of model parameters other than DISP on the apparent dispersion. From these rather exhaustive studies, the following guidance is offered:

(1) A spatial step or compartment size of 5.0 cm will mimic observed field effective dispersion quite well and should be used as an initial value.

(2) No fewer than 30 compartments should be used in order to minimize mass balance errors created by numerical dispersion.

(3) The DISP parameter should be set to 0.0 unless field data are available for calibration.

(4) If DISP calibration is attempted, the compartment size should be reduced to 1.0 cm to minimize the numerical dispersion.

(5) Equation 5-11 can be used to bound the values only should the need arise to increase dispersion beyond that produced by the numerical scheme.

If the user chooses the MOC algorithm to simulate advection transport, then numerical dispersion will be eliminated and a typical value for field-observed dispersion should be entered. Use of the MOC algorithm will result in increased model execution time.

DPN--Layer Depth in Each Horizon--
The DPN parameter allows the user to specify a different layer depth (i.e., compartment thickness) for each soil horizon. In general, a smaller DPN will generate more accurate results and provide greater spatial resolution, but will also consume more CPU time. From the volatilization viewpoint, a finer DPN in the top horizon is required for better estimation of the volatilization flux from the soil surface. In addition, since pesticide runoff is calculated from the surface layer, a smaller layer depth allows a better representation of surface-applied chemicals. For the surface horizon,

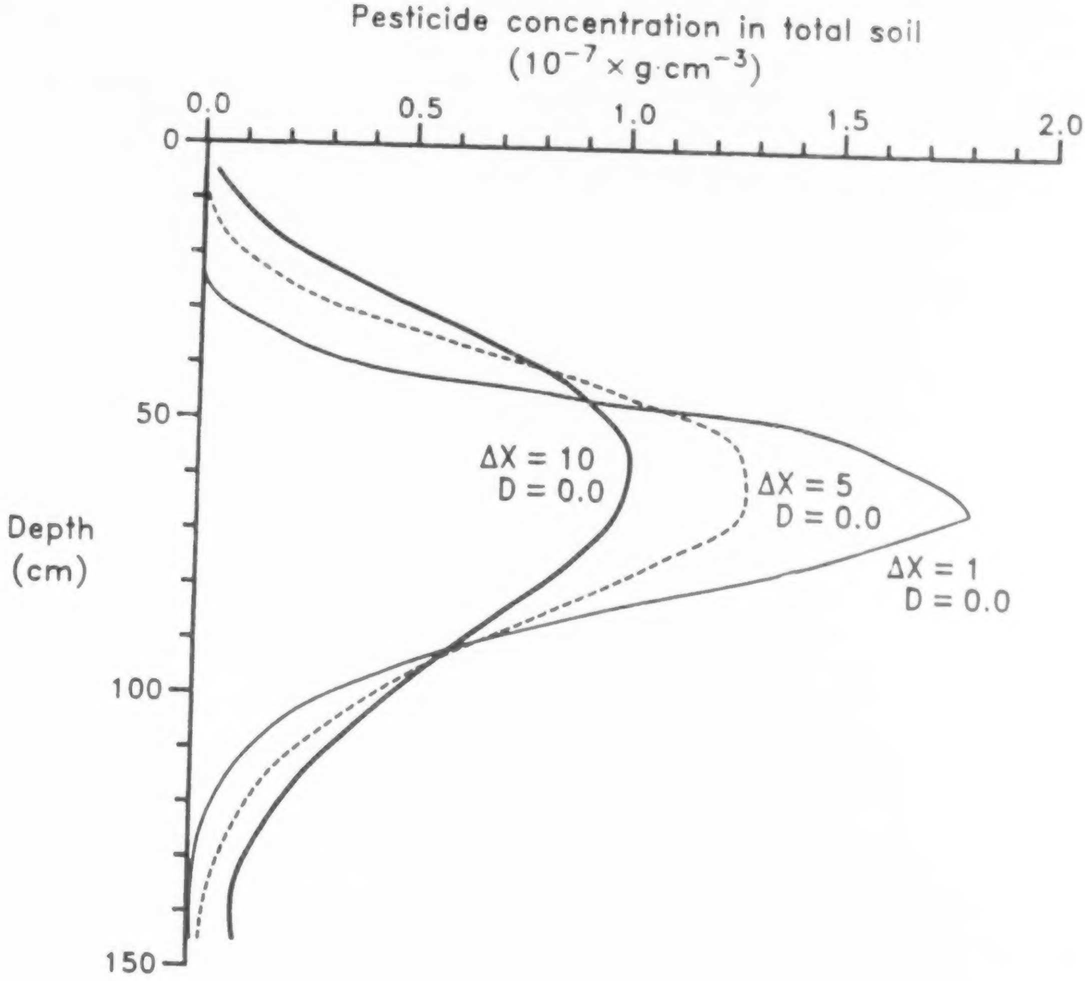

Figure 5.5. Numerical dispersion associated with space step (Δx).

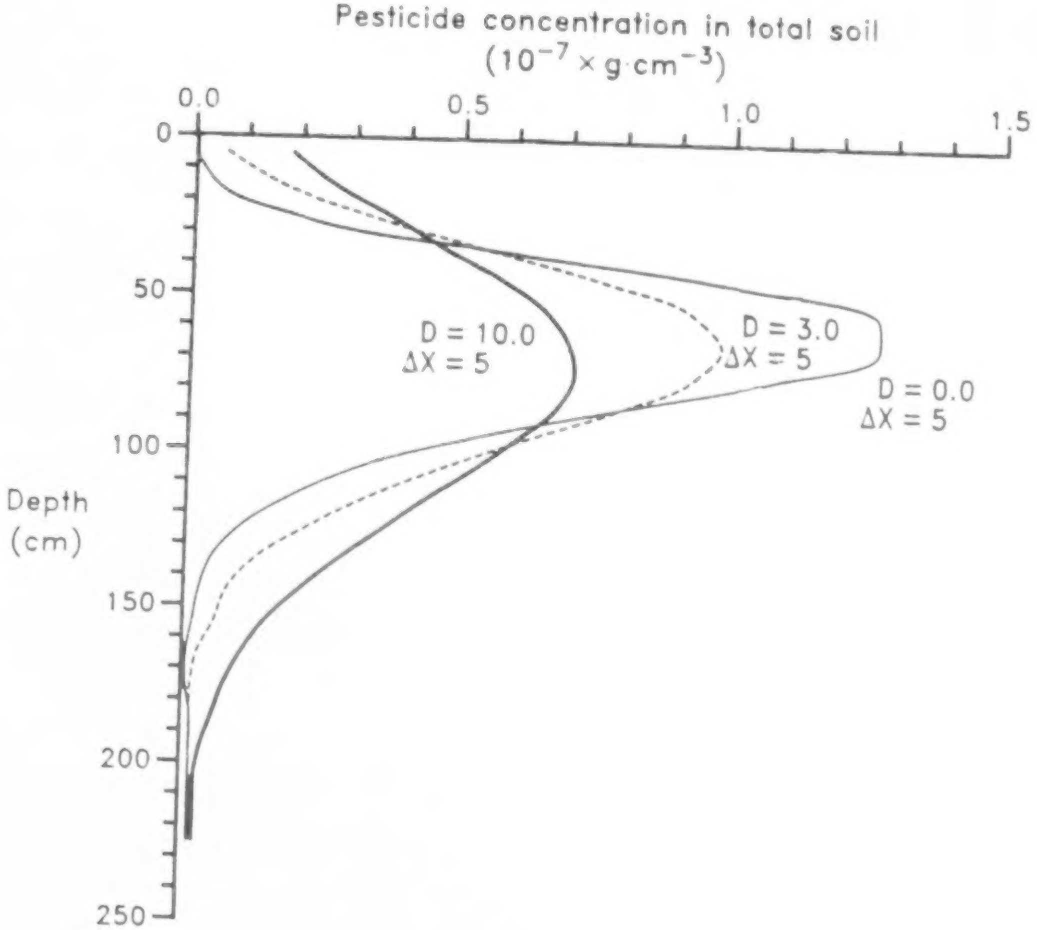

Figure 5.6. Physical dispersion (D) associated with advective transport. (Note: Numerical dispersion included).

DPN values in the range of 0.5 to 2.0 cm are recommended; a 1.0 cm value for DPN is commonly used. Smaller values down to 0.1 cm can be used for highly volatile compounds where volatilization is a major loss mechanism. For subsurface soil horizons, DPN values in the range of 5.0 to 30.0 cm are recommended depending on the spatial resolution needed at the lower depths.

APD, APM, IAPYR--Pesticide Application--
The use of PRZM requires the establishment of a pesticide application procedure. The user should follow the two steps described below in establishing representative application dates:

- establish an application period window covering the range of possible application dates

- adjust the application dates within the window so that application does not occur on a day immediately before, during, or immediately after a rainfall event (pesticides are not normally applied to a field with high moisture content or under conditions where the efficacy would be diminished).

5.2.4 Soil Temperature

ALBEDO--Soil Surface Albedo --
To simulate soil temperatures, ALBEDO values at start of each month must be specified. Soil surface albedo values depend on soil surface conditions during the period of simulation. As the surface condition changes, the albedo value changes accordingly. There is no simple procedure available that would estimate the albedo values for different surface conditions. The albedo values for some natural surface conditions are given in Table 5-20. A detailed procedure to calculate the albedo of soil surface covered with mulch and canopy is presented by Cruse et al. 1980.

ENMISS--Infrared Emissivity--
Most natural surfaces have an infrared emissivity lying between 0.9 and 0.99. Values for all natural surfaces are not well known, but it is usually close to unity. Specific values of emissivity for some natural surfaces are given in Table 5-21.

ZWIND--Height of Wind Speed Measuring Instrument--
The wind speed measuring anemometer is usually fixed at 10 meters (30 feet) above the ground surface. But this height may be different at some stations such as at class A weather stations where the anemometer may be attached to the evaporation pan. The correct value for ZWIND can be obtained from the meteorological data reports for the station whose data is used in the simulation.

BBT--Bottom Boundary Temperature--
In order to simulate soil temperature, BBT values at start of each month must be specified. The BBT soil temperature for shallow core depths may vary significantly with time throughout the year. For deep cores, the BBT will be relatively constant. Average monthly soil temperature values at core depth can be estimated from the climatological data reports published by NOAA,

Table 5-20. ALBEDO FACTORS OF NATURAL SURFACES FOR SOLAR RADIATION*

Surface	Reflectivity
Fresh Dry Snow	0.80-0.90
Clean, Stable Snow Cover	0.60-0.75
Old and Dirty Snow Cover	0.30-0.65
Dry Salt Cover	0.50
Lime	0.45
White Sand, Lime	0.30-0.40
Quartz Sand	0.35
Granite	0.15
Dark Clay, Wet	0.02-0.08
Dark Clay, Dry	0.16
Sand, Wet	0.09
Sand, Dry	0.18
Sand, Yellow	0.35
Bare Fields	0.12-0.25
Wet Plowed Field	0.05-0.14
Newly Plowed Field	0.17
Grass, Green	0.16-0.27
Grass, Dried	0.16-0.19
Grass, High Dense	0.18-0.20
Prairie, Wet	0.22
Prairie, Dry	0.32
Stubble Fields	0.15-0.17
Grain Crops	0.10-0.25
Alfalfa, Lettuce, Beets, Potatoes	0.18-0.32
Coniferous Forest	0.10-0.15
Deciduous Forest	0.15-0.25
Forest with Melting Snow	0.20-0.30
Yellow Leaves (fall)	0.33-0.36
Desert, Dry Soils	0.20-0.35
Desert, Midday	0.15
Desert, Low Solar Altitude	0.35
Water (0 to 30°)[a]	0.02
Water (60°)[a]	0.06
Water (85°)[a]	0.58

* References

Van Wijk, W.R. 1963. Physics of Plant Environment, p. 87. North-Holland Publishing Co., Amsterdam.

Brutsaert, W. 1982. Evaporation into the Atmopshere: Theory, History, and Applications. D. Reidel Publishing Co., Dordrecht, Holland.

[a] angle of solar incidence.

Table 5-21. EMISSIVITY VALUES FOR NATURAL SURFACES AT NORMAL TEMPERATURES*

Surface	Emissivity
Sand (dry-wet)	0.95-0.98
Mineral Soil (dry-wet)	0.95-0.97
Peat (dry-wet)	0.97-0.98
Firs	0.97
Tree Vegetation	0.96-0.97
Grassy Vegetation	0.96-0.98
Leaves	0.94-0.98
Water	0.95
Snow (old)	0.97
Snow (fresh)	0.99

* References

Van Wijk, W.R. 1963. Physics of Plant Environment, p. 87. North-Holland Publishing Co., Amsterdam.

Brutsaert, W. 1982. Evaporation into the Atmosphere: Theory, History, and Applications, D. Reidel Publishing Co., Dordrecht, Holland.

Department of Commerce. Depending on the core depth used in the simulation, the average temperature of shallow groundwater, as shown in Figure 5.7, may be used to estimate the BBT values.

THCOND and VHTCAP--Thermal Conductivity and Volumetric Heat Capacity of Soil Horizon--
If the user chooses to have the model simulate the soil temperature profile and sets the IDFLAG to zero, then the thermal conductivity and heat capacity values for each soil horizon must be specified. Representative values for some soil types are given in Table 5-22. Note that the value of THCOND is entered in PRZM in units of cal cm^{-1} $°C^{-1}$ day^{-1}, therefore the values in Table 5-22 should be multiplied by 86,400.

If IDFLAG = 1, thermal conductivity and heat capacity are calculated from soil composition (% sand, % clay, % OC), and the thermal properties of the soil components and water, based on the method in de Vries (1963).

SPT--Initial Soil Temperature Profile--
To simulate the soil temperature profile, initial SPT values for each soil horizon must be specified. Since PRZM is often used for long periods of simulation, the initial temperature profile will not have any significant effect on the predicted temperature profile after a few days or weeks of simulation unless the core is deep. Lower horizons in the core should be assigned values corresponding approximately to parameter BBT.

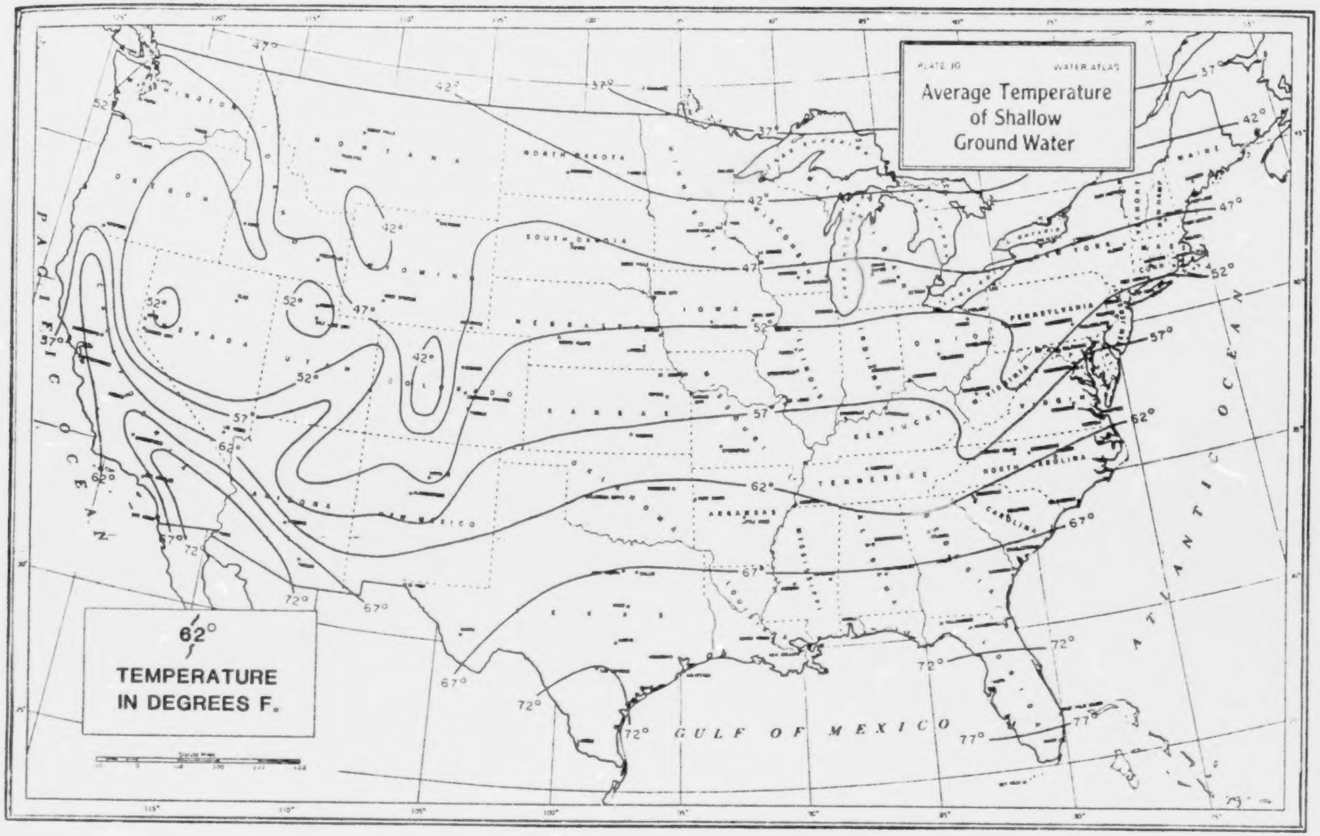
PLATE 10
WATER ATLAS
Average Temperature of Shallow Ground Water
62°
TEMPERATURE IN DEGREES F.
37°
42°
47°
52°
57°
62°
67°
72°
77°
PACIFIC OCEAN
ATLANTIC OCEAN
GULF OF MEXICO

Figure 5.7. Average temperature of shallow groundwater.

Table 5-22. THERMAL PROPERTIES OF SOME SOIL AND REFERENCE MATERIALS*

Material	Water Content (%)	Heat Capacity (cal cm^{-3} °C^{-1})	Thermal Cond. (cal cm^{-1}°C^{-1}sec^{-1})
Clay		1.44	0.00288
Light Soil w/Roots		0.09	0.00027
Wet Sandy Soil		0.64	0.0064
Dead Air		0.000312	0.00005
Hudson River Sand	4.5	0.2	0.0091
	18.1	0.336	0.03
Podunk Fine Sandy Loam	6.6	0.221	0.0012
	20.2	0.371	0.0026
Leonardtown Silt Loam	9.0	0.316	0.0018
	18.4	0.338	0.0021
Muck Soil	23.0	0.251	0.00076
	59.0	0.321	0.00108
Yolo Clay	0.0	0.236	0.0014
	29.0	0.72	0.0083
Granite Sandy Loam	0.0	0.291	0.0017
	22.7	0.706	0.0071
Fine Calcareous Loam	0.0	0.175	0.00079
	24.4	0.430	0.0048
Granitic Sand	0.0	0.269	0.00137
	13.1	0.636	0.0108
Barns Loam	5.1	0.29	0.00041
	26.0	0.35	0.00086
Chester Loam	2.0	0.32	0.00045
	13.4	0.37	0.00087
Herman Sandy Loam	1.3	0.30	0.00049
	13.4	0.37	0.00087
Kalkaska Loamy Sand	0.8	0.32	0.0006
	5.7	0.37	0.00124
Northway Silt Loam	6.6	0.384	0.0013
	22.5	0.636	0.0025
Fairbanks Silty Clay Loam	12.3	0.436	0.002
	25.4	0.625	0.0028
Dakota Sandy Loam	1.9	0.269	0.00059
	4.9	0.483	0.0054
Black Cotton Soil		0.336	0.00037

* References

Rosenberg, N.J. 1974. Microclimate: The Biological Environment, p. 105. Wiley - Interscience, New York.

Kilmer, V.J. 1982. Handbook of Soils and Climate in Agriculture. CRC Press, Inc. Boca Raton, Florida.

5.2.5 Soils Parameters

The amount of available moisture in the soil is affected by such properties as temperature and humidity, soil texture and structure, organic matter content, and plant characteristics (rooting depth and stage of growth). The moisture remaining in a soil after "gravity drainage" has ceased is known as field capacity. The moisture content in a soil below which plants cannot survive is called the wilting point. The wilting point, which varies among specific soils is influenced by colloidal material and organic matter, but most soils will have a similar wilting point for all common plants.

The PRZM model simulates soil water retention in the context of these bulk soil properties. Drainage of "excess water" is simulated as a simple daily value or as a daily rate. Most specific model parameters can be input directly by the user and some can be internally estimated given certain related soil properties as inputs.

THEFC, THEWP--Moisture Holding Capacity--

Field capacity (THEFC) and wilting point (THEWP) are required as user inputs. Often these soil-water properties have been characterized and values can be found from soils data bases. Where such data are not available, one of the three estimation methods given below can be used. Method one requires the textural properties (percent sand, silt, and clay), organic matter content (%), and bulk density (g cm^{-3}) of a specific soil. Method two utilizes a soil texture matrix for estimating soil water content if only the sand (%) and clay (%) contents are known. Method three provides mean field capacity and wilting points if only the soil texture is known.

Method 1 (also done within the code if THFLAG = 1)

The regression equation from Rawls and Brakensiek (1982) is used to estimate the matric water potential for various soils:

$$\theta_x = a + [b * \mathrm{SAND}(\%)] + [c * \mathrm{CLAY}(\%)] + [d * \mathrm{ORGANIC\ MATTER}(\%)] + [e * \mathrm{BULK\ DENSITY}\ (\mathrm{g\ cm^{-3}})] \tag{5-12}$$

where

θ_x = water retention $cm^3\ cm^{-3}$ for a given matric potential (field capacity = -0.33 bar and wilting point = -15.0 bar)

a-e = regression coefficients

Step 1. From Table 5-23 find the matric potential for field capacity and wilting point (-0.33 bar and -15.0 bar).

Table 5-23. COEFFICIENTS FOR LINEAR REGRESSION EQUATIONS FOR PREDICTION OF SOIL WATER CONTENTS AT SPECIIC MATRIC POTENTIALS[a]

Matric Coefficient	Intercept a	Sand (%) b	Clay (%) c	Organic Matter (%) d	Bulk Density (g cm^{-3}) e	R^2
-0.20	0.4180	-0.0021	0.0035	0.0232	-0.0859	0.75
-0.33	0.3486	-0.0018	0.0039	0.0228	-0.0738	0.78
-0.60	0.2819	-0.0014	0.0042	0.0216	-0.0612	0.78
-1.0	0.2352	-0.0012	0.0043	0.0202	-0.0517	0.76
-2.0	0.1837	-0.0009	0.0044	0.0181	-0.0407	0.74
-4.0	0.1426	-0.0007	0.0045	0.0160	-0.0315	0.71
-7.0	0.1155	-0.0005	0.0045	0.0143	-0.0253	0.69
-10.0	0.1005	-0.0004	0.0044	0.0133	-0.0218	0.67
-15.0	0.0854	-0.0004	0.0044	0.0122	-0.0182	0.66

[a] Rawls, W. J., U.S. Department of Agriculture, Agricultural Research Service, Beltsville, MD. Personal Communication.

Step 2. For each matric potential, find the regression coefficients (a-e) that are required in the Rawls and Brakensiek equation (e.g., for -0.33 potential, coefficients a-e are 0.3486, -0.0018, 0.0039, 0.0228, and -0.0738).

Step 3. For any given soil (example: Red Bay Sandy Loam where sand (%), 72.90; clay (%), 13.1; organic matter (%), 0.824; and bulk density (g cm^{-3}), 1.70) solve the equation for the -0.33 and -15.0 potential. For this example, THEFC = 0.170, THEWP = 0.090.

Method 2

Use Figure 5.8 for estimating the field capacity and Figure 5.9 for estimating the wilting point of any soil, given the percent sand and clay.

Step 1. Example: Red Bay Sandy Loam (field capacity). Find the percent sand across the bottom of Figure 5.8 (i.e., 73.0)

Step 2. Find the percent clay of the soil along the side of the triangle (i.e., 13.0).

Step 3. Locate the point where the two values intersect on the triangle and read the field capacity by interpolating between the contour lines, THEFC = 0.17.

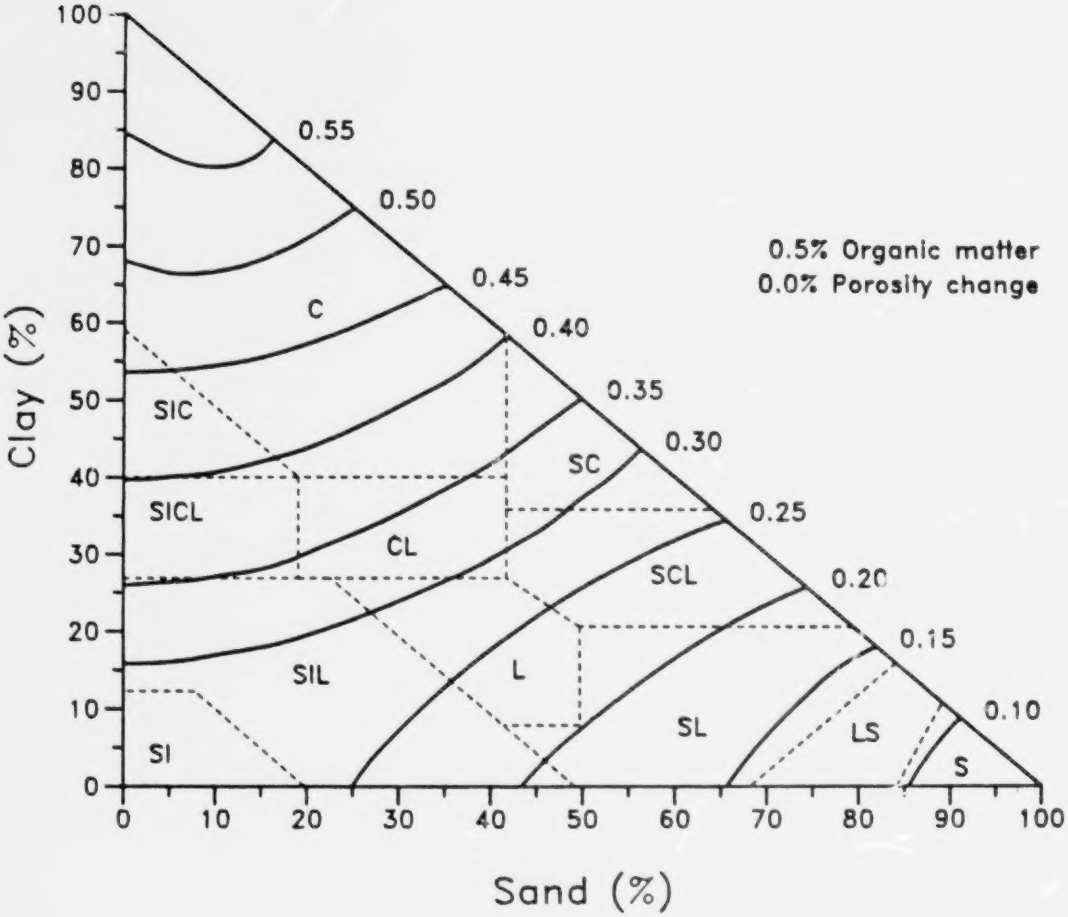

Figure 5.8. 1/3-bar soil moisture by volume. (provided by Dr. Walter J. Rawls, U.S. Department of Agriculture, Agricultural Research Service, Beltsville, Maryland).

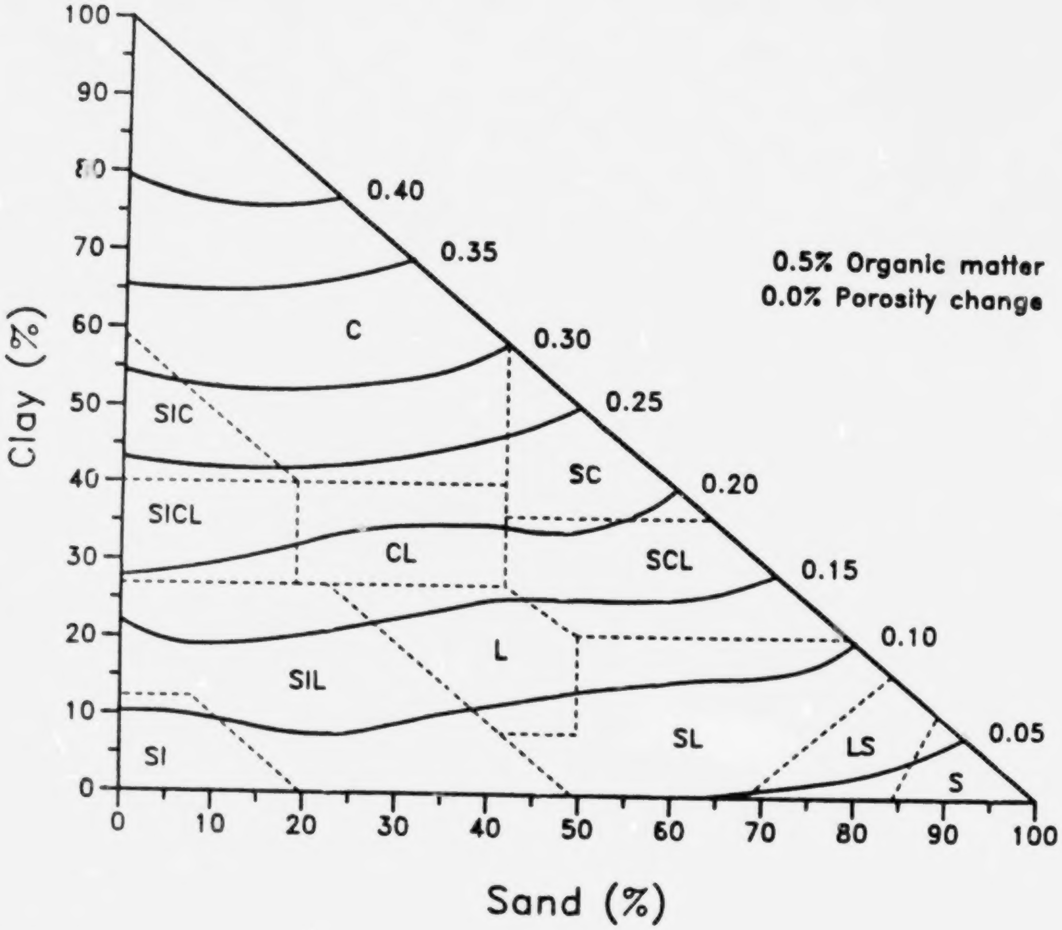

Figure 5.9. 15-bar soil moisture by volume. (provided by Dr. Walter J. Rawls, U.S. Department of Agriculture, Agricultural Research Service, Beltsville, Maryland).

Step 4. Follow Steps 2-4 for wilting point using Figure 5-9. THEWP = 0.09.

Method 3

Step 1. Use Table 5-24 to locate the textural class of the soil of choice.

Step 2. After locating the textural class, read the mean field capacity and wilting point potentials ($cm^3\ cm^{-3}$), to the right of the textural class. Example: Sandy loam. The mean field capacity (THEFC) and wilting point (THEWP) potentials are 0.207 and 0.095, respectively.

Guidance for estimating distributional properties for THEFC and THEWP is given in Tables 5-25 and 5-26. These tables show the arithmetic means and coefficients of variation for Hydrologic Groups A, B, C and D soils with depth. Also shown is the type of distribution which is most appropriate. Jury (1985) indicates overall CV for wilting point water content (15 bar tension) to be lower, at 24 percent. The values in the tables would tend to be more appropriate for regional assessments, whereas a lower value, such as that reported by Jury, would be more appropriate for single fields. He also indicates that the most appropriate distribution for static soil properties such as these is the normal.

Table 5-27 presents correlation coefficients between organic matter, field capacity, and wilting point for different soil strata and hydrologic groups, for use in Monte Carlo analyses.

Correlation coefficients between field capacity, and wilting point have moderate to high values ranging from 0.64 to 0.85 (Carsel et al. 1988).

BD--Bulk Density and Field Saturation--
Soil bulk density (BD) is required in the basic chemical transport equations of PRZM and is also used to estimate moisture saturation values. Values for BD can be input directly. When such data are not available for the site of interest, methods have been developed for their estimation. Two methods are provided for estimating BD of various soils. Method one requires the textural properties (percent sand, clay, and organic matter). Method two uses mean bulk density values if only the soil texture is known. The following steps provide procedures for estimating bulk density.

Method 1 (Also done within the code if BDFLAG = 1)

A procedure from Rawls (1983) is used to estimate bulk density for any given soil, provided the percent sand, clay, and organic matter contents are known. Example: Marlboro fine sandy loam--sand 80.0%, clay 5.0%, and organic matter 0.871%. Using the following equation:

Table 5-24. HYDROLOGIC PROPERTIES BY SOIL TEXTURE[a]

Texture Class	Range of Textural Properties (Percent) Sand	Silt	Clay	Water Retained at -0.33 Bar Tension $cm^3\ cm^{-3}$	Water Retained at -15.0 Bar Tension $cm^3\ cm^{-3}$
Sand	85-100	0-15	0-10	0.091[b] (0.018 - 0.164)[c]	0.033[b] (0.007 - 0.059)[c]
Loamy Sand	70-90	0-30	0-15	0.125 (0.060 - 0.190)	0.055 (0.019 - 0.091)
Sandy Loam	45-85	0-50	0-20	0.207 (0.126 - 0.288)	0.095 (0.031 - 0.159)
Loam	25-50	28-50	8-28	0.270 (0.195 - 0.345)	0.117 (0.069 - 0.165)
Silt Loam	0-50	50-100	0-28	0.330 (0.258 - 0.402)	0.133 (0.078 - 0.188)
Sandy Clay Loam	45-80	0-28	20-35	0.257 (0.186 - 0.324)	0.148 (0.085 - 0.211)
Clay Loam	20-45	15-55	28-50	0.318 (0.250 - 0.386)	0.197 (0.115 - 0.279)
Silty Clay Loam	0-20	40-73	28-40	0.366 (0.304 - 0.428)	0.208 (0.138 - 0.278)
Sandy Clay	45-65	0-20	35-55	0.339 (0.245 - 0.433)	0.239 (0.162 - 0.316)
Silty Clay	0-20	40-60	40-60	0.387 (0.332 - 0.442)	0.250 (0.193 - 0.307)
Clay	0-45	0-40	40-100	0.396 (0.326 - 0.466)	0.272 (0.208 - 0.336)

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[a] Rawls, W. J., D. L. Brakensiek, and K. E. Saxton. Estimation of Soil Water Properties. Transactions ASAE Paper No. 81-2510, pp. 1316 - 1320. 1982.

[b] Mean value.

[c] One standard deviation about the mean.

Table 5-25. DESCRIPTIVE STATISTICS AND DISTRIBUTION MODEL FOR FIELD CAPACITY (PERCENT BY VOLUME)

Stratum (m)	Sample Size	Original Data			CV (%)	Distribution Model		
		Mean	Median	s.d.		Transform	Mean	s.d.
Class A								
0.0-0.3	52	11.8	9.4	9.2	78	ln	2.25	0.65
0.3-0.6	50	9.6	8.1	7.9	82	ln	1.99	0.73
0.6-0.9	42	7.3	5.9	5.8	79	ln	1.73	0.73
0.9-1.2	39	7.1	5.8	5.0	70	ln	1.73	0.71
Class B								
0.0-0.3	456	19.5	19.1	8.3	42	s_U	0.316	0.13
0.3-0.6	454	18.8	18.8	7.4	39	s_U	0.311	0.12
0.6-0.9	435	18.7	18.7	7.1	39	s_U	0.298	0.11
0.9-1.2	373	17.5	17.5	7.6	43	s_U	0.288	0.12
Class C								
0.0-0.3	371	22.4	22.5	7.8	35	s_U	0.363	0.12
0.3-0.6	362	22.8	23.2	7.8	34	s_U	0.369	0.12
0.6-0.9	336	22.7	22.9	8.6	38	s_U	0.368	0.13
0.9-1.2	290	22.2	21.3	8.9	40	s_U	0.359	0.13
Class D								
0.0-0.3	230	24.1	24.2	9.1	38	s_U	0.387	0.14
0.3-0.6	208	26.1	26.3	9.3	36	s_U	0.419	0.14
0.6-0.9	178	25.0	25.6	8.2	33	s_U	0.403	0.13
0.9-1.2	146	24.1	24.4	8.1	33	s_U	0.390	0.12

CV = coefficient of variation
s.d. = standard deviation

Source: Carsel et al. (1988)

Table 5-26. DESCRIPTIVE STATISTICS AND DISTRIBUTION MODEL FOR WILTING POINT (PERCENT BY VOLUME)

Stratum (m)	Sample Size	Original Data				Distribution Model		
		Mean	Median	s.d.	CV (%)	Transform	Mean	s.d.
Class A								
0.0-0.3	118	4.1	3.1	3.4	82	ln	1.83	0.64
0.3-0.6	119	3.2	2.3	2.4	75	ln	0.915	0.71
0.6-0.9	113	2.9	2.1	2.3	81	s_B	3.32	0.88
0.9-1.2	105	2.6	1.9	2.3	87	s_B	3.43	0.92
Class B								
0.0-0.3	88	9.0	8.7	4.0	45	s_U	0.150	0.066
0.3-0.6	883	9.4	9.3	4.3	46	s_U	0.156	0.071
0.6-0.9	866	9.1	8.9	4.4	48	s_U	0.151	0.072
0.6-1.2	866	8.6	8.4	4.6	53	s_U	0.143	0.076
Class C								
0.3-0.3	678	10.8	10.4	5.1	48	s_U	1.63	0.62
0.3-0.6	677	12.2	12.1	5.6	46	s_U	0.202	0.091
0.6-0.9	652	12.2	11.9	6.0	49	s_U	0.201	0.096
0.9-1.2	582	11.8	11.5	5.7	48	s_U	0.194	0.092
Class D								
0.0-0.3	495	14.6	13.8	7.6	52	s_U	1.26	0.76
0.3-0.6	485	16.9	17.0	7.3	43	s_U	0.277	0.12
0.6-0.9	437	16.6	16.3	7.4	45	s_U	0.271	0.12
0.9-1.2	401	15.7	15.1	7.6	48	s_U	0.257	0.12

CV = coefficient of variation
s.d. = standard deviation

Source: Carsel et al. (1988)

Table 5-27. CORRELATIONS BETWEEN TRANSFORMED VARIABLES OF ORGANIC MATTER, FIELD CAPACITY, AND WILTING POINT

Stratum (m)	OM + WP		FC + OM		FC + WP	
	N	Corr.	N	Corr.	N	Corr.
Class A						
0.0-0.3	118	0.738	52	0.624	51	0.757
0.3-0.6	119	0.630	49	0.404	49	0.759
0.6-0.9	111	0.487	42	0.427	42	0.811
0.9-1.2	98	0.456	38	0.170	39	0.761
Class B						
0.0-0.3	877	0.545	459	0.609	455	0.675
0.3-0.6	870	0.372	446	0.384	450	0.639
0.6-0.9	844	0.375	419	0.336	429	0.714
0.9-1.2	780	0.392	347	0.412	370	0.762
Class C						
0.0-0.3	673	0.495	369	0.577	370	0.745
0.3-0.6	664	0.473	355	0.409	361	0.775
0.6-0.9	627	0.457	321	0.434	334	0.784
0.9-1.2	543	0.434	264	0.456	289	0.751
Class D						
0.0-0.3	488	0.538	228	0.496	226	0.847
0.3-0.6	472	0.434	201	0.454	204	0.845
0.6-0.9	420	0.456	171	0.369	174	0.782
0.9-1.2	384	0.415	137	0.106	145	0.687

OM = organic matter; WP = wilting point; FC = field capacity; N = sample size; Corr. = correlation.

Source: Carsel et al. 1988.

$$BD = \frac{100.0}{\frac{\%OM}{OMBD} + \frac{100.0 - \%OM}{MBD}} \qquad (5\text{-}13)$$

where

BD = soil bulk density, g cm^{-3}

OM = organic matter content of soil, %

OMBD = organic matter bulk density of soil, g cm^{-3} = 0.224

MBD = mineral bulk density, g cm^{-3}

NOTE: MBD must be entered if BDFLAG = 1.

Step 1. Locate the percent sand (80.0) along the bottom of Figure 5.10.

Step 2. Locate the percent clay (5.0) along the side of Figure 5.10.

Step 3. Locate the intersection point of the two values and read the mineral bulk density (1.55).

Step 4. Solve the Rawls equation for BD (e.g., 1.47).

Method 2

Step 1. Use Table 5-28 to locate the textural classification of the soil.

Step 2. Read mean bulk density for the general soil texture. Example: Sandy loam. The mean bulk density is 1.49 g cm^{-3}.

Table 5-29 shows distributional properties of bulk density information. The information given is categorized by Hydrologic Soil Group (A, B, C, D). The most appropriate distribution for this property is the normal (Jury 1985). Jury indicates slightly lower CVs, on the order of 9 percent. Values of CV in the table are more appropriate for regional simulations, whereas a value of 9-10% is more appropriate for a single field.

OC--Percent of Soil Organic Carbon--
Soil organic carbon (OC) is conventionally related to soil organic matter as %OC = %OM/1.724. Guidance on estimating percent organic matter is found in Table 5-30. Information is categorized by Hydrologic Soil Group and by depth. Also shown are coefficients of variation for each soil group and depth. Carsel et al. (1988) determined that the Johnson SB distribution provides the best fit to this data.

Rao and Wagenet (1985) and Nielsen et al. (1983) have reported that these values are often normally distributed. Carsel et al. (1988) have noted that organic carbon is weakly correlated with field capacity and wilting point

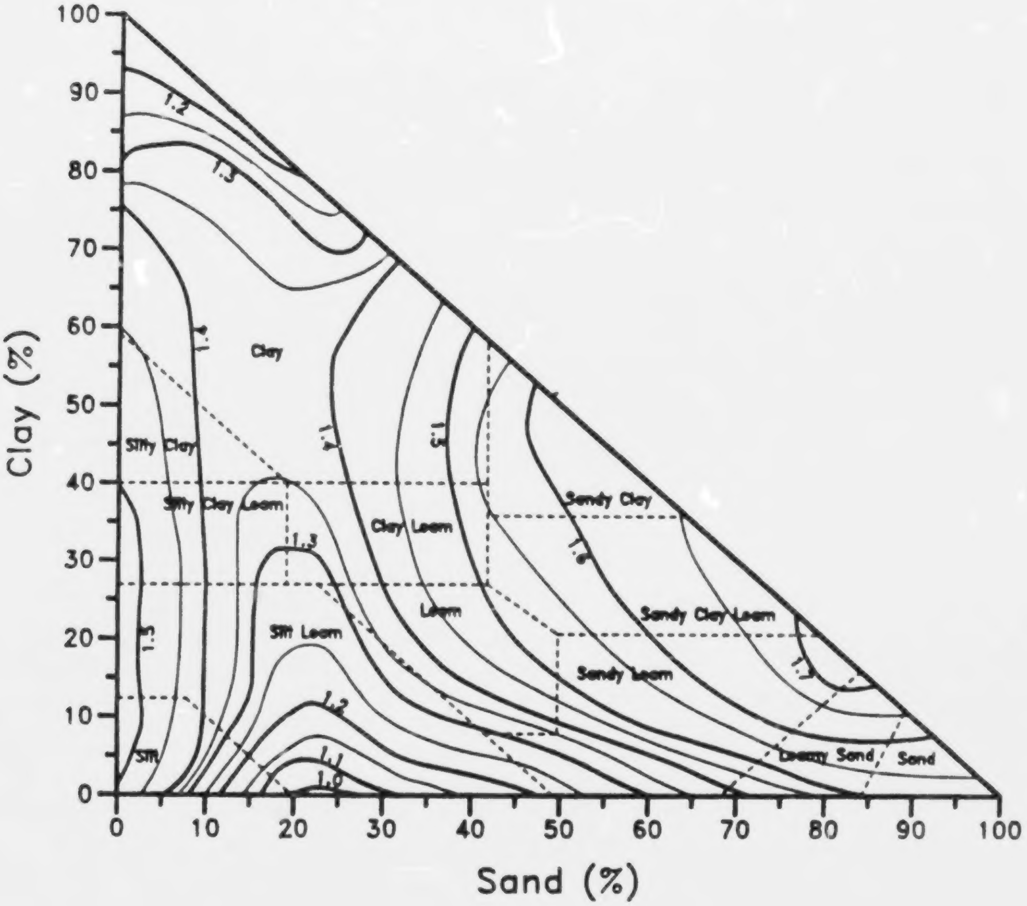


Figure 5.10. Mineral bulk density (gcm^{-3}). (provided by Dr. Walter J. Rawls, U.S. Department of Agriculture, Agricultural Research Service, Beltsville, Maryland).

water content with correlation coefficients ranging from 0.1 to 0.74. Strength of correlation decreases with depth, as shown previously in Table 5-27.

Table 5-28. MEAN BULK DENSITY (g cm^{-3}) FOR FIVE SOIL TEXTURAL CLASSIFICATIONS[a]

Soil Texture	Mean Value	Range Reported
Silt Loams	1.32	0.86 - 1.67
Clay and Clay Loams	1.30	0.94 - 1.54
Sandy Loams	1.49	1.25 - 1.76
Gravelly Silt Loams	1.22	1.02 - 1.58
Loams	1.42	1.16 - 1.58
All Soils	1.35	0.86 - 1.76

[a] Baes, C.F., III and R.D. Sharp. 1983. A Proposal for Estimation of Soil Leaching Constants for Use in Assessment Models. J. Environ. Qual. 12(1): 17-28.

AD--Soil Water Drainage Rate (for HSWZT = 1)--

The HSWZT flag indicates which drainage model is invoked for simulating the movement of recharging water. Drainage model 1 (HSWZT = 0) is for freely draining soils; drainage model 2 (HSWZT = 1) is for more poorly drained soils. For soils with infiltration rates of more than 0.38 cm hr^{-1} (associated with SCS hydrologic soils groups A, B, and some C), setting HSWZT = 0 is recommended. For soils with infiltration rates of less than 0.38 cm hr^{-1} (associated with groups D and some C) setting HSWZT = 1 is recommended.

The drainage rate parameter (AD), required when HSWZT = 1, is an empirical constant and dependent on both soil type and the number of compartments to be simulated. Although there is limited experience using this option, an analysis was performed to determine the best value for AD over a range of soil types on which agricultural crops are commonly grown. Each of three soil types was tested with a constant soil profile depth (125 cm). The profile was divided into a variable number of compartments and the optimum value of AD for each soil/compartment combination was obtained.

The analysis was performed by comparing the storage of water in the soil profile following the infiltration output from SUMATRA-1 (van Genuchten 1978). This model was used as "truth" because field data were lacking and SUMATRA-1 is theoretically rigorous. The amount of water moving out of the profile changed by only 1 - 2% over the range of compartments tested (15 - 40) for the three soils evaluated. Calibrating PRZM by comparison was accomplished and estimates of AD calculated. Suggested values of AD for clay

Table 5-29. DESCRIPTIVE STATISTICS FOR BULK DENSITY (g cm^{-3})

Stratum (m)	Sample Size	Mean	Median	s.d.	CV (%)
Class A					
0.0-0.3	40	1.45	1.53	0.24	16.2
0.3-0.6	44	1.50	1.56	0.23	15.6
0.6-0.9	38	1.57	1.55	0.16	10.5
0.9-1.2	34	1.58	1.59	0.13	8.4
Class B					
0.0-0.3	459	1.44	1.45	0.19	13.5
0.3-0.6	457	1.51	1.53	0.19	12.2
0.6-0.9	438	1.56	1.57	0.19	12.3
0.9-1.2	384	1.60	1.60	0.21	12.9
Class C					
0.0-0.3	398	1.46	1.48	0.22	15.0
0.3-0.6	395	1.58	1.59	0.23	14.5
0.6-0.9	371	1.64	1.65	0.23	14.2
0.9-1.2	326	1.67	1.68	0.23	14.0
Class D					
0.0-0.3	259	1.52	1.53	0.24	15.9
0.3-0.6	244	1.63	1.66	0.26	16.0
0.6-0.9	214	1.67	1.72	0.27	16.3
0.9-1.2	180	1.65	1.72	0.28	17.0

CV = coefficient of variation
s.d. = standard deviation

Source: Carsel et al. (1988)

Table 5-30. DESCRIPTIVE STATISTICS AND DISTRIBUTION MODEL FOR ORGANIC MATTER (PERCENT BY WEIGHT)

Stratum (m)	Sample Size	Original Data				Distribution Model[a]	
		Mean	Median	s.d.	CV (%)	Mean	s.d.
Class A							
0.0-0.3	162	0.86	0.62	0.79	92	-4.53	0.96
0.3-0.6	162	0.29	0.19	0.34	114	-5.72	0.91
0.6-0.9	151	0.15	0.10	0.14	94	-6.33	0.83
0.9-1.2	134	0.11	0.07	0.11	104	-6.72	0.87
Class B							
0.0-0.3	1135	1.3	1.1	0.87	68	-4.02	0.76
0.3-0.6	1120	0.50	0.40	0.40	33	-5.04	0.77
0.6-0.9	1090	0.27	0.22	0.23	84	-5.65	0.75
0.9-1.2	1001	0.18	0.14	0.16	87	-6.10	0.78
Class C							
0.0-0.3	838	1.45	1.15	1.12	77	-3.95	0.79
0.3-0.6	822	0.53	0.39	0.61	114	-5.08	0.84
0.3-0.9	780	0.28	0.22	0.27	96	-5.67	0.83
0.9-1.2	672	0.20	0.15	0.21	104	-6.03	0.88
Class D							
0.0-0.3	638	1.34	1.15	0.87	66	-4.01	0.73
0.3-0.6	617	0.65	0.53	0.52	80	-4.79	0.78
0.6-0.9	558	0.41	0.32	0.34	84	-5.29	0.82
0.9-1.2	493	0.29	0.22	0.31	105	-5.65	0.86

CV = coefficient of variation

s.d. = standard deviation

Source: Carsel et al. (1988)

[a] Johnson s_B transformation is used for all cases in this table.

loam, loamy sand, and sand as a function of the number of compartments are given in Figure 5.11.

5.2.6 Parameter Estimation for Irrigation

Guidance is provided below for estimating parameters simulating irrigation with PRZM.

IRTYPE--Selecting the Type of Irrigation--
The variable IRTYPE is used to indicate which type of irrigation is to be simulated, and should reflect agricultural practices in the region of interest. Table 5-31 lists conditions under which furrow, sprinkler, and flood irrigation are usually used. In general, furrow (IRTYPE = 1) and flood (IRTYPE = 2) irrigation are more commonly used in the West and Midwest, where topography is more level. Sprinklers (IRTYPE = 3,4) can be used in any type of terrain and for any crop, and are increasingly popular due to concerns about erosion from furrow- and flood-irrigated fields. Sprinklers are more expensive to install, but generally apply water more efficiently than do other irrigation methods.

PCDEPL--Fraction of Available Water Capacity Where Irrigation is Triggered--
The moisture level where irrigation is required is defined by the model user as fraction of the available water capacity. This fraction will depend upon the soil moisture-holding characteristics, the type of crop planted, and regional agricultural practices. In general, PCDEPL should range between 0.0 and 0.6, where a value of 0.0 indicates that irrigation begins when soil moisture drops to the wilting point, and 0.6 indicates the more conservative practice of irrigating at 60 percent of the available water capacity. Schwab et al. (1966) recommend values of PCDEPL ranging between 0.45 and 0.55.

FLEACH--Leaching Factor--
The leaching factor is used to specify the amount of water added by irrigation to leach salts from saline soil, and is defined as a fraction of the amount of water required to meet the soil water deficit. For instance, a value of 0.0 indicates no water is added for leaching, while a value of 0.25 indicates that 25 percent extra water is added to the irrigation water volume required to meet the soil water deficit.

RATEAP--Maximum Sprinkler Application Rate--
RATEAP is used to limit sprinkler applications to volumes that the sprinkler system is capable of delivering in a PRZM time step, and is defined as a maximum depth (cm) of water delivered per hour. Table 5-32 lists appropriate sprinkler delivery rates for different slopes and soil types; sprinkler systems designed for these conditions should be capable of supplying at least the amounts of water listed in Table 5-32. Other guidance for estimating maximum application rates can be found in industry specifications for different sprinkler systems.

Furrow Irrigation Parameters--The first set of furrow irrigation parameters define the flow characteristics and geometry of furrow channels. These parameters will generally depend upon soil characteristics and topography, with some variation occurring due to different local agricultural practices.

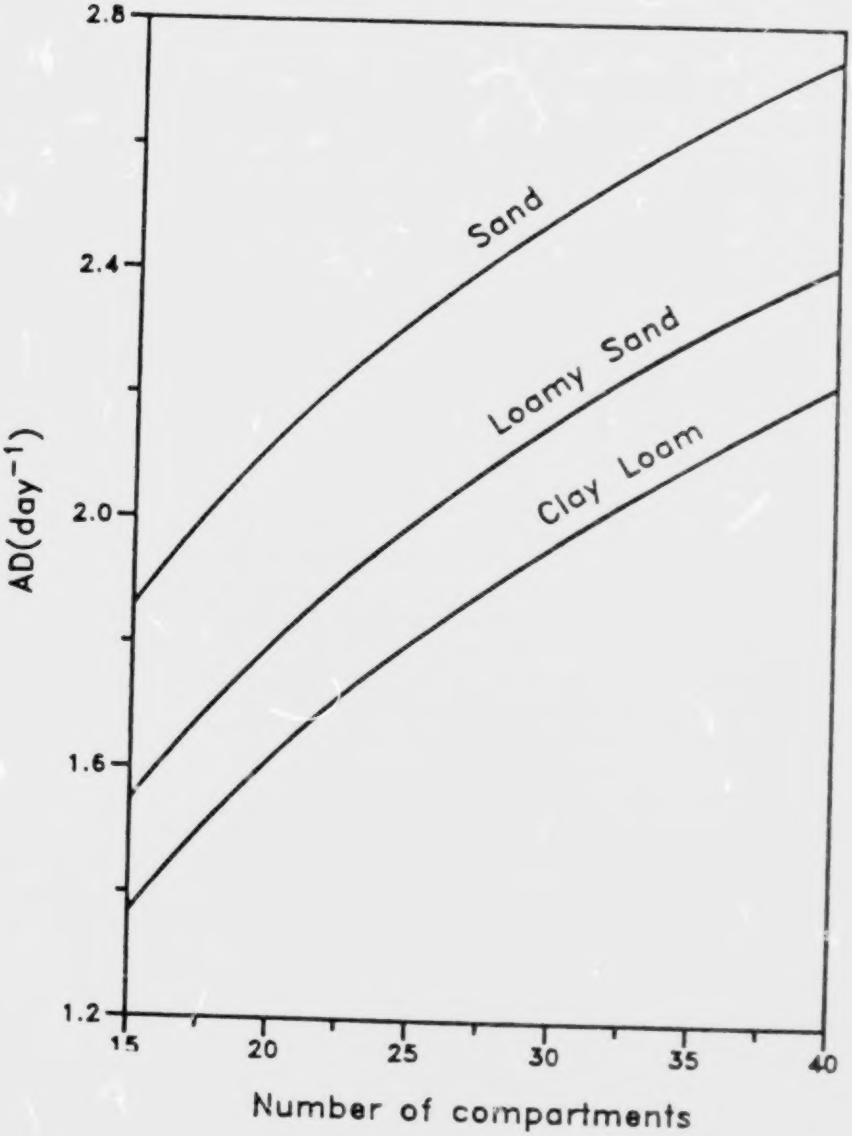


Figure 5.11. Estimation of drainage rate AD (day^{-1}) versus number of compartments.

Table 5-31. ADAPTATIONS AND LIMITATIONS OF COMMON IRRIGATION METHODS

Irrigation Method	Adaptations	Limitations
Furrow	Light, medium-and fine-textured soils; row crops.	Slopes up to 3 percent in direction of irrigation; row crops; 10 percent cross slope.
Sprinklers	All slopes; soils; crops.	High initial equipment cost; lowered efficiency in wind and hot climate.
Flood	Light, medium, and heavy soils.	Deep soils; high cost of land preparation; slopes less than 2 percent.

Source: Adapted from Todd (1970).

Table 5-32. WATER REQUIREMENTS FOR VARIOUS IRRIGATION AND SOIL TYPES

	Typical Application Rate (Inches/Hour) by Sprinklers				
	Slope (%)	Coarse Sandy Soils	Light Sandy Loam	Medium Silt Loam	Clay Loam Soils
Sprinkling	0-2	2.0	0.75	0.5	0.20
	2-5	2.0	0.75	0.5	0.20
	5-8	1.5	0.50	0.4	0.15
	8-12	1.0	0.40	0.3	

Source: Adapted from Todd (1970).

Typical values of these parameters for furrows described in the literature are listed in Table 5-33.

QO Flow Rate into a Single Furrow - QO is defined as the volume of water entering the furrow per unit time. Flow rates are usually set so that sufficient water reaches the end of the furrow without causing excessive erosion. Table 5-34 lists maximum non-erosive flow rates for various furrow channel slopes.

BT Bottom Width of Furrows - BT will depend mostly upon the type of equipment used to dig the furrow channels and the spacing between furrows.

Z Side Slope of Furrows - This parameter is defined as the slope of the channel walls, horizontal distance/vertical distance. Z will depend upon the cohesiveness of soils and the type of equipment used to dig the furrows. Table 5-35 lists suitable side slopes for different types of soils, with values ranging from 1.5 to 3.0 for unconsolidated materials.

SF Channel Slope - SF is determined by regional topography and the design grades of the furrows, and is defined as vertical drop in elevation per horizontal distance of the bed. Furrows are usually used only in relatively level terrain, with slopes no greater than .03 (Todd 1970). A few representative slopes are listed in Table 5-33.

EN Manning's Roughness Coefficient - Manning's roughness coefficient is a well-known measure of the resistance of open channels to flow. Chow (1959) suggests that values of EN range from .016 to .033 in excavated or dredged earth channels. Values for furrows listed in Table 5-33 range from .01 to .048. Table 5-36 lists values of EN suggested by the USDA Soil Conservation Service for drainage ditches with various values of hydraulic radius (defined as the flow area divided by the wetted perimeter).

XL Length of Furrow - XL will depend upon the size of the field and the local topography. Table 5-34 lists maximum furrow lengths for various soil textures, irrigation application depths, and furrow slopes.

The second set of furrow parameters are related to the infiltration characteristics of the soil, and are used in the Green-Ampt infiltration model:

KS Saturated Hydraulic Conductivity - This parameter represents the limiting infiltration rate when the soil column is saturated and suction pressure is no longer important. KS depends upon soil mineralogy, texture, and degree of compaction. Ranges of values for various unconsolidated materials are shown in Table 5-37. KS has also been correlated with SCS Hydrologic Soil Groups (Brakensiek and Rawls 1983); ranges of values for each soil group are shown in Table 5-38.

Table 5-33. REPRESENTATIVE FURROW PARAMETERS DESCRIBED IN THE LITERATURE

Reference	Location	Soil	Crop	Channel Slope	Flow Rate (m^3/s)	Furrow Length (m)	Bottom Widtn(cm)	Manning's Roughness Coefficient
Elliott et al. (1982)	Colorado	Clay loam Clay loam Loamy sand	Corn Corn Corn	.0044 .0092 - .0095 .0023 - .0025	.001 - .003 .00085 - .00096 .003 - .005	625 425 - 450 350	-- -- --	.02 - .03 .02 - .03 .02 - .03
Hall (1956)	--	Medium Textured	Corn	.005	----	200	--	.035
Fangmeier and Ramsey (1978)	Arizona	Fine sandy loam	None (test furrows)	.01	.0004 - .0018	9	--	.02 - .04
Karmeli et al. (1978)	Colorado	Clay loam	None	.0045	.0011	625	10 - 20	.01 - .048

Table 5-34. FURROW IRRIGATION RELATIONSHIPS FOR VARIOUS SOILS, SLOPES, AND DEPTHS OF APPLICATION

Soil Texture		Coarse				Medium				Fine			
		Depth of irrigation application (inches)											
Slope (percent)	Max allowable nonerosive furrow stream (gpm)	2	4	6	8	2	4	6	8	2	4	6	8
		Maximum allowable length of run (feet)											
.25	40	500	720	875	1,000	820	1,150	1,450	1,650	1,050	1,500	1,750	2,140
.50	20	345	480	600	680	560	800	975	1,120	730	1,020	1,250	1,460
.75	13	270	380	480	550	450	630	775	900	580	820	1,000	1,150
1.00	10	235	330	400	470	380	540	650	760	500	750	850	990
1.50	7	190	265	330	375	310	430	530	620	400	570	700	800
2.00	5	160	225	275	320	260	370	450	530	345	480	600	675
3.00	3	125	180	220	250	210	295	360	420	270	385	470	550
5.00	2	95	135	165	190	160	225	270	320	210	290	350	410

Source: Adapted from Todd (1970).

Table 5-35. SUITABLE SIDE SLOPES FOR CHANNELS BUILT IN VARIOUS KINDS OF MATERIALS

Material	Side slope
Rock	Nearly vertical
Muck and peat soils	¼:1
Stiff clay or earth with concrete lining	½:1 - 1:1
Earth with stone lining, or earth for large channels	1:1
Firm clay or earth for small ditches	1½:1
Loose sandy earth	2:1
Sandy loam or porous clay	3:1

Source: Adapted from Chow (1959).

Table 5-36. VALUE OF "N" FOR DRAINAGE DITCH DESIGN

Hydraulic radius (ft)	EN
< 2.5	0.040 - 0.045
2.5 - 4.0	0.035 - 0.040
4.0 - 5.0	0.030 - 0.035
> 5.0	0.025 - 0.030

Source: Adapted from U.S. Dept. of Agric. Soil Conservation Service.

Table 5-37. REPRESENTATIVE PERMEABILITY RANGES FOR SEDIMENTARY MATERIALS

Material	Hydraulic Conductivity (m/s)	Material	Hydraulic Conductivity (m/s)
Clay	10^{-12} - 10^{-9}	Very fine sand	10^{-7} - 10^{-4}
Silty clay	10^{-12} - 10^{-9}	Find sand	10^{-6} - 10^{-3}
Sandy clay	10^{-11} - 10^{-8}	Medium sand	10^{-5} - 10^{-3}
Silty clay loam	10^{-10} - 10^{-7}	Coarse sand	10^{-5} - 10^{-2}
Sandy loam sand	10^{-9} - 10^{-6}	Gravel and sand	10^{-5} - 10^{-2}
Silt	10^{-9} - 10^{-6}	Gravel	10^{-5} - 10^{-2}
Silt loam	10^{-9} - 10^{-6}	Sandstone	10^{-6} - 10^{-3}
Loam	10^{-9} - 10^{-6}	Limestone*	10^{-7} - 10^{-4}
Sandy loam	10^{-8} - 10^{-7}	Shale	10^{-7} - 10^{-4}

* Excluding cavernous limestone; Source: Adapted from Todd (1970).

Table 5-38. VALUES OF GREEN-AMPT PARAMETERS FOR SCS HYDROLOGIC SOIL GROUPS

SCS Hydrologic Soil Group	Saturated Hydraulic[a] Conductivity K_s (cm hr^{-1})	Suction Parameter HF (cm)
A	1.0 - 10.0	10
B	0.60 - 1.0	10 - 20
C	0.20 - 0.60	15 - 10
D	0.005 - 0.20	20 - 150

Source: Adapted from Brakensiek and Rawls (1983).

[a] Also see Table 5-30.

HF Suction Parameter - HF represents water movement due to suction in unsaturated soils, and has units of length (meters). As in the case of KS, HF has been correlated with SCS Hydrologic Soil Groups (Brakensiek and Rawls 1983); ranges of values for each soil group are shown in Table 5-38.

5.3 VADOFT PARAMETERS

Input data for variably saturated flow simulations include the following:

(1) System Geometry

- Soil column dimensions (L)

(2) Porous Medium Properties

- Saturated hydraulic conductivity, K_s (LT^{-1})
- Specific storage, S_s (L^{-1})
- Effective porosity, ϕ

(3) Constitutive Relationships for Variably Saturated Flow

- Tabulated data of k_{rw} versus S_w, or values of parameters of analytic expressions for k_{rw} versus S_w
- Tabulated data of S_w versus ψ, or values of parameters of analytic expressions for S_w versus ψ.

(4) Initial and Boundary Conditions

- Prescribed values of pressure head, $\bar{\psi}$ (L)
- Prescribed values of nodal fluid flux (infiltration rate), I (LT^{-1})

Input data for the transport model include the following:

(1) System Geometry

- Soil column dimensions (L)

(2) Porous Medium Properties

- Longitudinal dispersivity α_L, (L)
- Molecular diffusion coefficients, D^* (L^2T^{-1})
- Effective porosity, ϕ

(3) Properties of Solute Species

- Decay coefficient, λ (T^{-1})
- Retardation coefficient, R

(4) Darcy Velocity, V ($L\ T^{-1}$)

(5) Water Saturation, S_w

(6) Initial and Boundary Conditions

- Prescribed value of concentration, c_o ($M\ L^{-3}$)
- Prescribed value of solute flux, Vc_o ($M\ L^{-2}\ T^{-1}$)

Guidance for certain of these parameters is given in the following paragraphs.

Saturated Hydraulic Conductivity--

Saturated hydraulic conductivity represents the rate at which a porous medium can transmit water under saturated conditions. Table 5-39 gives representative values for various soil types. Also note the values of the coefficient of variation in column three. These CVs are for many soils nationwide which fall into this texture category. CVs for a single soil are likely to be lower. Jury (1985) gives a CV of 120% for this parameter which may be more representative. The most likely shape for the distribution is lognormal.

Table 5-39. DESCRIPTIVE STATISTICS FOR SATURATED HYDRAULIC CONDUCTIVITY ($cm\ hr^{-1}$)

	Hydraulic Conductivity (K_s)*			
Soil Type	$\bar{x}$	s	CV	n
Clay**	0.20	0.42	210.3	114
Clay Loam	0.26	0.70	267.2	345
Loam	1.04	1.82	174.6	735
Loamy Sand	14.59	11.36	77.9	315
Silt	0.25	0.33	129.9	88
Silt Loam	0.45	1.23	275.1	1093
Silty Clay	0.02	0.11	453.3	126
Silty Clay Loam	0.07	0.19	288.7	592
Sand	29.70	15.60	52.4	246
Sandy Clay	0.12	0.28	234.1	46
Sandy Clay Loam	1.31	2.74	208.6	214
Sandy Loam	4.42	5.63	127.0	1183

* n = Sample size, $\bar{x}$ = Mean, s = Standard deviation, CV = Coefficient of variation (percent)

** Agricultural soil, less than 60 percent clay

Source: Carsel and Parrish (1988).

Soil-Water Characteristic Data--
The user is allowed two options: either to input these data as a set of paired functions (water saturation [S_w] vs. relative conductivity [K_{rw}] and pressure head [ψ] vs. water saturation [S_w] or to input parameters of the analytic expressions for these functions in the code. The parameterization of the latter functions is discussed here.

In order to provide a linkage for these parameters to widely known or easily obtained soils data (such as soil texture), Carsel and Parrish (1988) fit these analytic functions to data from soils all over the U.S. and tabulated corresponding parameter values by texture. These are shown in Table 5-40. The required parameters are α, β, and γ of the van Genuchten model (see Section 3, Volume I). Mean values of these parameters are shown along with CVs for each by soil texture. Other parameters required to use these relationships are the air entry pressure head (ψ_a) and the residual water content (θ_r). The air entry pressure head is normally taken to be zero. Values of the residual water content are given in Table 5-41 along with their respective CVs. Table 5-42 from Carsel and Parrish (1988) shows the types of probability density functions used to fit the sample distributions of saturated hydraulic conductivity, residual water content, and van Genuchten parameters α and β.

Note that γ is related to β by the relationship:

$$\gamma = 1 - 1/\beta \qquad (5\text{-}14)$$

In addition, Table 5-43 gives the correlations between these parameters by soil textural classification.

Specific Storage--
For unsaturated zone flow, the specific storage is set to 0.

Effective Porosity--
The mean values of saturation water content (θ_s) and residual water content (θ_r) shown in Table 5-41 can be used to estimate effective porosity. The saturation water content (θ_s) is equal to the total porosity of the soil. The effective porosity can be roughly approximated as the difference of θ_s and θ_r in Table 5-41. CVs for soil texture categories are also shown in Table 5-41. According to Jury (1985) the normal distribution is an appropriate probability density function for this parameter.

Longitudinal Dispersivity--
The user should refer to the discussion of the dispersion coefficient (cm^2 day^{-1}) in Section 5.2.3. Dispersion coefficients are calculated by the model as the product of the seepage velocity and the dispersivity input by the user. In the absence of site-specific values it is recommended that the dispersivity be chosen as one-tenth of the distance of the flow path or:

Table 5-40. DESCRIPTIVE STATISTICS FOR VAN GENUCHTEN WATER RETENTION MODEL PARAMETERS, α, β, and γ (Carsel and Parrish 1988)

Soil Type	Parameter α, cm^{-1}				Parameter β				Parameter γ			
	$\bar{X}$	SD	CV	N	$\bar{X}$	SD	CV	N	$\bar{X}$	SD	CV	N
Clay[a]	0.008	0.012	160.3	400	1.09	0.09	7.9	400	0.08	0.07	82.7	400
Clay Loam	0.019	0.015	77.9	363	1.31	0.09	7.2	364	0.24	0.06	23.5	364
Loam	0.036	0.021	57.1	735	1.56	0.11	7.3	735	0.36	0.05	13.5	735
Loamy Sand	0.124	0.043	35.2	315	2.28	0.27	12.0	315	0.56	0.04	7.7	315
Silt	0.016	0.007	45.0	88	1.37	0.05	3.3	88	0.27	0.02	8.6	88
Silt Loam	0.020	0.012	64.7	1093	1.41	0.12	8.5	1093	0.29	0.06	19.9	1093
Silty Clay	0.005	0.005	113.6	126	1.09	0.06	5.0	374	0.09	0.05	51.7	374
Silty Clay Loam	0.010	0.006	61.5	641	1.23	0.06	5.0	641	0.19	0.04	21.5	641
Sand	0.145	0.029	20.3	246	2.68	0.29	20.3	246	0.62	0.04	6.3	246
Sandy Clay	0.027	0.017	61.7	46	1.23	0.10	7.9	46	0.18	0.06	34.7	46
Sandy Clay Loam	0.059	0.038	64.6	214	1.48	0.13	8.7	214	0.32	0.06	53.0	214
Sandy Loam	0.075	0.037	49.4	1183	1.89	0.17	9.2	1183	0.47	0.05	10.1	1183

$\bar{X}$ = Mean, SD = Standard Deviation, CV = Coefficient of Variation (percent), N = Sample size

[a] Agricultural Soil, Clay 60 percent

Table 5-41. DESCRIPTIVE STATISTICS FOR SATURATION WATER CONTENT (θ_s) AND RESIDUAL WATER CONTENT (θ_r)

Soil Type	Saturation Water Content (θ_s)				Residual Water Content (θ_r)			
	Statistic*							
	$\bar{x}$	s	CV	n	x	s	CV	n
Clay**	0.38	0.09	24.1	400	0.068	0.034	49.9	353
Clay Loam	0.41	0.09	22.4	364	0.095	0.010	10.1	363
Loam	0.43	0.10	22.1	735	0.078	0.013	16.5	735
Loamy Sand	0.41	0.09	21.6	315	0.057	0.015	25.7	315
Silt	0.46	0.11	17.4	82	0.034	0.010	29.8	82
Silt Loam	0.45	0.08	18.7	1093	0.067	0.015	21.6	1093
Silty Clay	0.36	0.07	19.6	374	0.070	0.023	33.5	371
Silty Clay Loam	0.43	0.07	17.2	641	0.089	0.009	10.6	641
Sand	0.43	0.06	15.1	246	0.045	0.010	22.3	246
Sandy Clay	0.38	0.05	13.7	46	0.100	0.013	12.9	46
Sandy Clay Loam	0.39	0.07	17.5	214	0.100	0.006	6.0	214
Sandy Loam	0.41	0.09	21.0	1183	0.065	0.017	26.6	1183

* n = Sample size, $\bar{x}$ = Mean, s = standard deviation, CV = coefficient of variation (percent)

** Agricultural soil, less than 60 percent clay.

Source: Carsel and Parrish, 1988

$$\alpha_L = 0.1\ x_v \qquad (5\text{-}15)$$

where

x_v = the thickness of the vadose zone.

Molecular Diffusion--
See the discussion in Section 5.2.3.

Pesticide Decay Coefficients--
See the discussion in Section 5.2.3.

Retardation Factors--
In VADOFT, in contrast to PRZM, the user inputs the retardation factor R instead of the distribution coefficient, K_D(cm^3 g^{-1}). The retardation factor is defined for saturated conditions in the input:

Table 5-42. STATISTICAL PARAMETERS USED FOR DISTRIBUTION APPROXIMATION

Soil Texture**	Hydraulic Variable	Transformation	Limits of Variation		Mean	Estimated* Standard Deviation	D****	Truncation Limits on Transformed Variable	
			A	B					
S	K_s	SB	0.0	70.0	-0.39387	1.15472	0.045		
S	θ_r	LN	0.0	0.1	-3.11765	0.22369	0.053		
S	α	SB	0.0	0.25	0.37768	0.43895	0.050		
S	β	LN	1.5	4.0	0.97813	0.10046	0.063		
SL	K_s	SB	0.0	30.0	-2.49047	1.52854	0.029		
SL	θ_r	SB	0.00	0.11	0.38411	0.70011	0.034		
SL	α	SB	0.00	0.25	-0.93655	0.76383	0.044		
SL	β	LN	1.35	3.00	0.63390	0.08162	0.039		
LS	K_s	SB	0.0	51.0	-1.26908	1.40000	0.036		
LS	θ_r	SB	0.0	0.11	0.07473	0.56677	0.043		
LS	α	NO	0.0	0.25	0.12354	0.04345	0.027		
LS	β	SB	1.35	5.00	-1.11095	0.30718	0.070		
SIL	K_s	LN	0.0	15.0	-2.18691	1.49414	0.046		
SIL	θ_r	SB	0.0	0.11	0.47752	0.58156	0.073		
SIL	α	LN	0.0	0.15	-4.09937	0.55542	0.083		
SIL	β	SB	1.0	2.0	-0.37036	0.52557	0.104		
SI	K_s	LN***	0.0	2.0	-2.20	0.7000	0.168	-2.564	-0.337
SI	θ_r	ND***	0.0	0.09	0.042	0.0145	0.089	0.013	0.049
SI	α	NO	0.0	0.1	0.01688	0.00611	0.252		
SI	β	NO	1.2	1.6	1.37815	0.03729	0.184		
C	K_s	SB	0.0	5.0	-5.75949	2.32884	0.122		
C	θ_r	SU**	0.0	0.15	0.44537	0.28178	0.058	0.0065	0.834
C	α	SB**	0.0	0.15	-4.14805	1.29310	0.189	-5.01	0.912
C	β	LN**	0.9	1.4	0.00021	0.11800	0.131	0.00	0.315
SIC	K_s	LN	0.0	1.0	-5.68562	1.31421	0.205		
SIC	θ_r	NO	0.0	0.14	0.06971	0.02337	0.058		
SIC	α	LN	0.0	0.15	-5.65849	0.58445	0.164		
SIC	β	SB	1.0	1.4	-1.28378	0.82074	0.069		
SC	K_s	LN	0.0	1.5	-4.04036	2.01721	0.130		
SC	θ_r	SB	0.0	0.12	1.72496	0.70000	0.078		
SC	α	LN	0.0	0.15	-3.76810	0.56322	0.127		
SC	β	LN	1.0	1.5	0.20209	0.07788	0.100		
SICL	K_s	SB	0.0	3.5	-5.31256	1.61775	0.049		
SICL	θ_r	NO	0.0	0.115	0.08871	0.00937	0.056		
SICL	α	SB	0.0	0.15	-2.75043	0.60529	0.082		
SICL	β	NO	1.0	1.5	1.23640	0.06130	0.082		

Table 5-42. STATISTICAL PARAMETERS USED FOR DISTRIBUTION APPROXIMATION (concluded)

Soil Texture**	Hydraulic Variable	Transformation	Limits of Variation A	Limits of Variation B	Mean	Estimated* Standard Deviation	D****	Truncation Limits on Transformed Variable	
CL	K_s	SB***	0.0	7.5	-5.87171	2.92220	0.058	-8.92	2.98
CL	θ_r	SU	0.0	0.13	0.67937	0.06005	0.061		
CL	α	LN	0.0	0.15	-4.21897	0.71389	0.052		
CL	β	SB	1.0	1.6	0.13248	0.72498	0.035		
SCL	K_s	SB	0.0	20.0	-4.03718	1.84976	0.047		
SCL	θ_r	SB***	0.0	0.12	1.65387	0.43934	0.077	0.928	2.94
SCL	α	SB	0.0	0.25	-1.37920	0.82327	0.048		
SCL	β	LN	1.0	2.0	0.38772	0.08645	0.043		
L	K_s	SB	0.0	15.0	-3.71390	1.77920	0.019		
L	θ_r	SB	0.0	0.12	0.63872	0.48709	0.064		
L	α	SB	0.0	0.15	-1.27456	0.78608	0.039		
L	β	SU	1.0	2.0	0.53169	0.09948	0.036		

* For distribution of transformed variables.

** S = sand, SL = sandy loam, LS = loamy sand, SIL = silty loam, SI = silt, C = clay, SIC = silty clay, SC = sandy clay, SICL = silty clay loam, CL = clay loam, SCL = sandy clay loam, L = loam.

*** Truncated form of the distribution.

**** Kolmogorov-Smirnov test statistic.

Source: Carsel and Parrish, 1988.

Table 5-43. CORRELATIONS AMONG TRANSFORMED VARIABLES PRESENTED WITH THE FACTORED COVARIANCE MATRIX*

	K_s	θ_r	α	β
Silt **(n = 61)				
K_s	0.5349258	-0.0015813	0.0030541	0.0128700
θ_r	-0.204	0.0075771	0.0000021	-0.0145118
α	0.984	-0.200	0.0005522	0.0144376
β	0.466	-0.610	0.551	0.0133233
Clay (n = 95)				
K_s	1.9614077	0.0701669	0.5645309	0.0475514
θ_r	0.972	0.0170159	-0.0798488	-0.0142394
α	0.948	0.890	0.1716520	0.0021973
β	0.908	0.819	0.910	0.0164640
Silty Clay (n = 123)				
K_s	1.2512845	0.0082067	0.3143268	0.3674505
θ_r	0.949	0.0027392	0.0404171	-0.0858769
α	0.974	0.964	0.0608834	0.0660396
β	0.908	0.794	0.889	0.1305065
Sandy Clay (n = 46)				
K_s	2.0172105	0.8827527	0.5391195	0.0756103
θ_r	0.939	0.3241979	0.0634106	0.0035688
α	0.957	0.937	0.1501651	-0.0010668
β	0.972	0.928	0.932	0.0178225
Sand (n = 237)				
K_s	1.0370702	-0.1092256	0.3276629	0.0805436
θ_r	-0.515	0.1816914	0.2583835	-0.0471785
α	0.743	0.119	0.1429585	-0.0013674
β	0.843	-0.858	0.298	0.0167064
Sandy Loam (n = 1145)				
K_s	1.6026856	-0.1529235	0.0372713	0.2108253
θ_r	-0.273	0.5378436	0.0174500	-0.1943369
α	0.856	0.151	0.0142626	0.0193794
β	0.686	-0.796	0.354	0.1084945
Loamy Sand (n = 313)				
K_s	1.4754063	-0.2005639	0.0372713	0.2108253
θ_r	-0.359	0.5215473	0.0174500	-0.1943369
α	0.986	-0.301	0.0142626	0.0193794
β	0.730	-0.590	0.354	0.1084945

Table 5-43. CORRELATIONS AMONG TRANSFORMED VARIABLES PRESENTED WITH THE FACTORED COVARIANCE MATRIX* (concluded)

	K_s	θ_r	α	β
Silt Loam (n = 1072)				
K_s	1.4754063	-0.02005639	0.5245489	0.3525548
θ_r	-0.359	0.5215473	0.0300399	-0.1696100
α	0.986	-0.301	0.0820163	0.2341768
β	0.730	-0.590	0.775	0.1583593
Silty Clay Loam (n = 591)				
K_s	1.6177521	0.0056509	0.5116521	0.0486478
θ_r	0.724	0.0053780	0.0475299	-0.0089569
α	0.986	0.777	0.0731704	0.0080399
β	0.918	0.549	0.911	0.0171716
Clay Loam (n = 328)				
K_s	1.9200165	0.0395603	0.5886263	0.5417671
θ_r	0.790	0.0307122	-0.0619715	-0.1536351
α	0.979	0.836	0.1060875	0.0653030
β	0.936	0.577	0.909	0.1159401
Sandy Clay Loam (n = 212)				
K_s	1.8497610	0.1020156	0.7838769	0.0766289
θ_r	0.261	0.3775754	0.1223451	-0.0305588
α	0.952	0.392	0.2198684	-0.0078559
β	0.909	-0.113	0.787	0.0155766
Loam (n = 664)				
K_s	1.4083953	-0.0995016	0.6110671	0.0545016
θ_r	0.204	0.4775039	0.0727710	-.0545793
α	0.982	-0.086	0.0926351	0.0256843
β	0.632	-0.748	0.591	0.0288861

* Entries in the lower triangular portion of the matrix are sample Pearson product-moment correlations given to three decimal places. The diagonal and upper triangular entries form the triangular Cholesky decomposition of the sample covariance matrix.

** N = Sample size.

Source: Carsel and Parrish, 1988.

$$R = 1 + \frac{K_d \rho}{\theta_s} \qquad (5\text{-}16)$$

and is adjusted internally for values of $\theta < \theta_s$. In the above equation, ρ is the soil bulk density (g cm^{-3}) and θ_s is the saturation water content (cm^3 cm^{-3}). In making this calculation, the user should directly use the value for ρ, if known. If necessary, ρ can be approximated according to:

$$\rho = 2.65\ (1 - \theta_s) \qquad (5\text{-}17)$$

The CV of the retardation factor, R, can be computed knowing the uncertainties in K_d, ρ and θ_s (Taylor 1982). The fractional uncertainties add to give an upper bound error on R (CV_{max}) or are combined as a root mean square for independent random errors. Thus,

$$CV_{max} = (CV_{\theta_s} + CV_{K_d} + CV_{\rho}) \qquad (5\text{-}18)$$

or

$$CV = 100\ [(CV_{\theta_s}/100)^2 + (CV_{K_d}/100)^2 + (CV_{\rho}/100)^2]^{1/2} \qquad (5\text{-}19)$$

The uncertainty in the value of K_d will depend upon whether it is measured, calculated as the product of K_{oc} and % organic carbon, and whether the K_{oc} is calculated from a surrogate parameter such as octanol water partition coefficient (K_{ow}) or solubility (s). Directly measured values would obviously have lower CVs. Assuming that K_d is calculated from a measured soluble concentration, then it is possible that the CV would be on the order of 60 - 130% (Jury 1985). For K_d derived from K_{ow} or solubility, the CV could be on the order of 1000%.

5.4 SAFTMOD PARAMETERS

Data required for the groundwater flow simulation include values of the saturated hydraulic conductivity and specific storage of each aquifer and aquitard material, the geometry and configuration of the flow region, as well as initial and boundary conditions associated with the flow equation. Data required for the simulation of solute transport include values of longitudinal and transverse dispersivities and porosity, retardation and decay constants, and values of Darcy velocity components, as well as initial and boundary conditions associated with the transport equation.

Input data of the flow model include the following:

(1) System Geometry

- Horizontal and vertical dimensions, including layering and other heterogeneities (L)

(2) Porous-Medium Properties

For each aquifer,

- Hydraulic conductivity component, K_{11} ($L\ T^{-1}$)
- Hydraulic conductivity component, K_{22} ($L\ T^{-1}$)
- Hydraulic conductivity component, K_{33} ($L\ T^{-1}$)
- Specific storage, S_s (L^{-1})
- Specific yield, S_y

For each aquitard,

- Hydraulic conductivity, K' ($L\ T^{-1}$)
- Specific storage, S_s (L^{-1})

(3) Initial Boundary Conditions

- Prescribed values of pressure head, $\bar{h}$ (L)
- Prescribed values of nodal fluid flux, Q_n ($L^3\ T^{-1}$)
- Recharge rate, I ($L\ T^{-1}$)

Input data of the transport model include the following:

(1) System Geometry

- Horizontal and vertical dimensions, including layering and other heterogeneities (L)

(2) Porous-Medium Properties

For each aquifer,

- Longitudinal dispersivity, α_L (L)
- Transverse dispersivity, α_T (L)
- Molecular diffusion coefficient, D_o ($L^2\ T^{-1}$)
- Effective porosity, ϕ

For each aquitard,

- Diffusion coefficient, D' ($L^2\ T^{-1}$)
- Effective porosity, ϕ'

(3) Solute Properties

- Decay constant, λ (T^{-1})
- Retardation in aquifer, R
- Retardation in aquitard, R'

(4) Darcy velocity components of groundwater, V_1 and V_2 ($L\ T^{-1}$)

(5) Initial and Boundary Conditions

- Initial values of concentration, c_o ($M\ L^{-3}$)
- Prescribed values of concentration, $\bar{c}$ ($M\ L^{-3}$)
- Prescribed values of solute flux, $\dot{M}$ ($M\ T^{-1}$)

Hydraulic Conductivity--
In the absence of site-specific measurements, the hydaulic conductivity can be estimated using Tables 5-37 and 5-39. An alternative, though often a poor one, is to calculate the hydraulic conductivity by means of an approximate functional relationship. One such relationship, the Karman-Cozney equation (Bear 1979), can be expressed as:

$$K_s = \frac{\rho g}{\mu} \frac{\phi^3}{(1-\phi)^2} \frac{d^2}{1.8} \qquad (5\text{-}20)$$

where

K_s = the hydraulic conductivity (cm sec^{-1})
ρ = the density of water (Kg m^{-3})
g = acceleration due to gravity (m sec^{-2})
μ = the dynamic viscosity of water (N sec m^{-2})
d = mean particle diameter (cm) and
ϕ = the effective porosity (dimensionless)

In Eq. 5-20 the constant 1.8 includes a unit conversion factor. Both the density of water (ρ) and the dynamic viscosity of water (μ) are functions of temperature. Values can be computed using regression equations presented in CRC (1981). Note that at 15°C, the value of [$\rho g/1.8\mu$] is about 478.

Ranges of values for various aquifer materials can be found in Freeze and Cherry (1979). K_s is probably log-normally distributed, having a range of values from 0.0001 to 0.48 cm sec^{-1} (Federal Register 1986).

Specific Storage--

Specific storage (L^{-1}) can be calculated from the expression:

$$S_s = \rho g \ (\alpha + \theta_s \beta) \tag{5-21}$$

where

S_s = the specific storage (L^{-1})
ρ = fluid density ($M \ L^{-3}$)
g = the acceleration of gravity ($L \ T^{-2}$)
α = compressibility of the aquifer ($L \ T^2 \ M^{-1}$)
θ_s = saturated water content or porosity ($L^3 \ L^{-3}$)
β = compressibility of water ($L \ T^2 \ M^{-1}$)

The value of β can be taken as $4.4*10^{-10}$ $m^2 \ N^{-1}$ (Freeze and Cherry 1979). The value of α for various aquifer materials may be taken from the following data:

Material	Aquifer Compressibility, α ($m^2 \ N^{-1}$)
Clay	10^{-6} - 10^{-9}
Sand	10^{-7} - 10^{-9}
Gravel	10^{-8} - 10^{-10}
Jointed Rock	10^{-8} - 10^{-10}
Sound Rock	10^{-9} - 10^{-11}

The term ρg is equal to $9.8*10^{-3}$ $N \ m^{-3}$ and can be considered constant. Therefore, S_s is a function of the aquifer type and porosity:

$$S_s = 9.8*10^3 \ (\alpha + 4.4*10^{-10} \ \theta_s) \tag{5-22}$$

A typical value for a predominantly sandy aquifer ($\alpha = 10^{-8}$, $\theta_s = 0.30$) would be $9.9*10^{-5}$ m^{-1}.

Dispersion Coefficients--

The model computes the longitudinal and either lateral or vertical dispersion coefficients as the product of the seepage velocity and longitudinal (α_L), transverse (α_T) or vertical (α_V) dispersivities. A literature review indicated generalized theory to describe dispersivities, although a strong dependence on scale has been noted (EPRI 1985). In the absence of user specified values, the following guidance is given.

Based on the values presented in the Federal Register (1986), the longitudinal and transverse dispersivities are:

$$\alpha_L = 0.1\ x_r \tag{5-23}$$

$$\alpha_T = \frac{\alpha_L}{3.0} \tag{5-24}$$

where x_r is the distance from the source to the receptor well. The vertical dispersivity, α_V, can be assumed to be uniformly distributed in the range of .025 to .1 of the longitudinal dispersivity. Distributional properties of the longitudinal and transverse dispersivities are unknown.

Saturated Water Content (Porosity)--
In the absence of a user-specified distribution for the saturated water content (porosity), it can be calculated from the particle diameter using the following empirical relationship (Federal Register 1986):

$$\theta_s = 0.261 - 0.0385\ \ln(d) \tag{5-25}$$

where d = the mean particle diameter [cm]. Given a typical range of d (Federal Register 1986) of 0.0004 to 0.10 cm for aquifer materials, θ_s would be 0.30 to 0.56 if Equation 5-25 is used. Its distribution is probably normal or uniform.

Effective Porosity/Specific Yield--
In the absence of site specific information, the effective porosity or specific yield can be approximated using Figure 5.12.

Solute Decay--
Degradation of solute may be the result of many factors. General guidance for chemical degradation is given in Section 5.2.3. If hydrolysis is the principal degradation pathway, then the following procedures may be used to establish hydrolysis rates.

The acid-catalyzed, neutral, and base-catalyzed hydrolysis rates are all influenced by groundwater temperature. This effect is often quantified using the Arrhenius equation, that yields:

$$K^{T}_{a,n,b} = K^{T_r}_{a,n,b}\ \exp\left[\ E_a/R_g \left(\frac{1}{T_r + 273} - \frac{1}{T + 273}\right)\right] \tag{5-26}$$

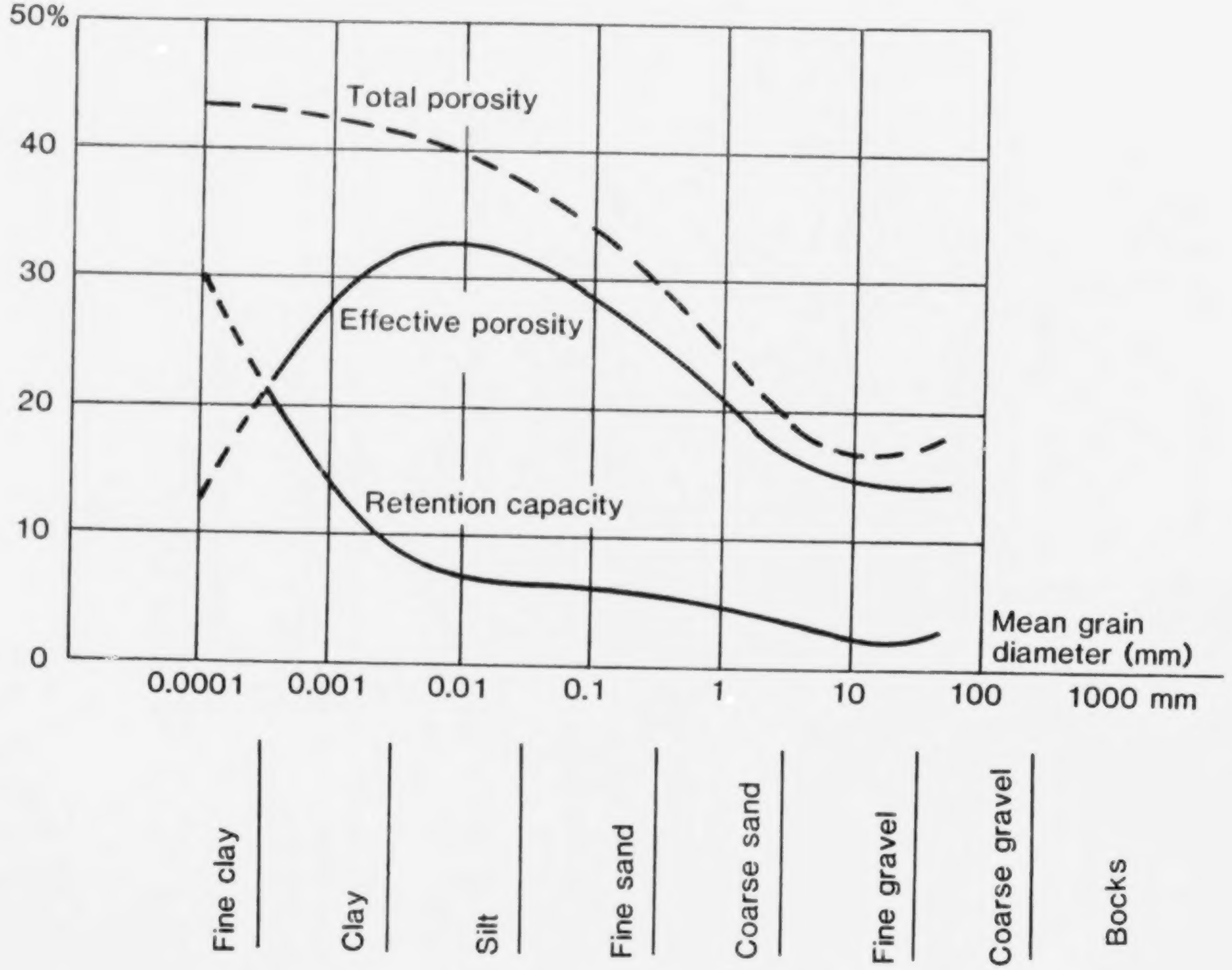


Figure 5.12. Porosity components as a function of grain size. (After de Marsily, 1986).

where

T = temperature of the groundwater [°C]

T_r = reference temperature [°C]

$K_{a,b}^{T}$ and $K_{a,b}^{T_r}$ = the second-order acid- and base-catalysis hydrolysis rates at temperature T and T_r respectively [$\ell \text{mole}^{-1} \text{yr}^{-1}$]

$K_n^{T_r}$ and K_n^{T} = the neutral hydrolysis rate at temperatures T_r and T respectively [yr^{-1}]

R_g = universal gas constant [1.987E-3 Kcal $°\text{C}^{-1}$ mole^{-1}]

E_a = Arrhenius activation energy [Kcal mole^{-1}]

Note that using the generic activation energy of 20 Kcal/mole recommended by Wolfe (1985), the factor E_a/R_g has a value of about 10,000.

The acid-catalyzed, base-catalyzed, and neutral hydrolysis rate constants can be combined (Mill et al., 1983) to yield the composite, first-order, dissolved phase hydrolysis rate:

$$\lambda_1 = K_a^T [H^+] + K_n^T + K_b^T [OH^-] \qquad (5\text{-}27)$$

where

$[H^+]$ = the hydrogen ion concentration [mole ℓ^{-1}]

$[OH^-]$ = the hydroxyl ion concentration [mole ℓ^{-1}]

Note that $[H^+]$ and $[OH^-]$ can both be computed from the pH of the aquifer, i.e.,

$$[H^+] = 10^{-pH} \qquad (5\text{-}28)$$

$$[OH^-] = 10^{-(14-pH)} \qquad (5\text{-}29)$$

For the case of sorbed phase hydrolysis, evidence suggests that base neutralized hydrolysis can be neglected and that the acid neutralized hydrolysis rate is enhanced by a factor of α. Thus, the effective sorbed phase decay rate can be expressed as:

$$\lambda_2 = \alpha K_a^T [H^+] + K_n^T \qquad (5\text{-}30)$$

where α = acid-catalysis hydrolysis rate enhancement factor for sorbed phase with a typical value of 10.0.

Retardation Factor--
As discussed in Section 5.3, the retardation factor is a function of the distribution coefficient (K_d), bulk density (ρ), and saturation water content (θ_s):

$$R = 1 + \frac{K_d \rho}{\theta_s} \tag{5-32}$$

If values of bulk density ρ are not known, they can be approximated using equation 5-17.

The relationship most suited for relating the chemical distribution coefficient, K_d, to soil or porous medium properties is discussed in detail by Karichoff (1984). In the absence of user-specified values, hydrophobic binding is assumed to dominate the sorption process. For this case, the distribution coefficient can be related directly to soil organic carbon using:

$$K_d = K_{oc} f_{oc} \tag{5-31}$$

where

K_{oc} = normalized distribution coefficient for organic carbon

f_{oc} = fractional organic carbon in the saturated zone

The discussion of the magnitude of the coefficient of variation for the distribution of K_d also applies here. The distribution of f_{oc} used for waste sites from all over the U.S. has a range of 0.001 to 0.01, a mean of 0.00315, and a standard deviation of 0.0003 (Woodward-Clyde Consultants, 1988). It is lognormally distributed with a transformed mean of -5.76 and a transformed standard deviation of 3.17 (Federal Register 1986). Section 6.3.3 of Volume I discusses the lognormal distribution and provides equations for calculating the transformed mean and standard deviation parameters.

SECTION 6

EXAMPLE PROBLEMS

The example problem presented in this section is for the simulation of fate and transport of the pesticide aldicarb on Long Island. The section opens with a brief description of the site, and proceeds to discuss the values of various model parameters utilized in the simulation. Results are then presented, which are compared to field-measured data.

6.1 THE PHYSICAL SETTING

This problem has previously been simulated by Lafleur et al. (1981). The following description of the site hydrogeology and local setting is taken from that report.

> Long Island extends from New York City eastward about 120 miles. It is underlain by consolidated bedrock, which in turn is overlain by a wedge-shaped mass of unconsolidated sedimentary materials. The top of the bedrock, which is at or near the land surface in the northern part of the island, slopes to the southeast to depths of about 2000 feet below sea level at the south shore. The general hydrologic situation has been reviewed by Cohen, Franke and Foxworthy (1968) and will not be repeated in detail.
>
> The materials that overlie the bedrock and constitute the groundwater reservoir consist of Pleistocene deposits and Cretaceous unconsolidated fluvial and deltaic deposits of gravel, sand, silt, and clay. Groundwater in the uppermost part of the saturated zone, mainly the upper glacial aquifer, but locally also in the Magothy aquifer, is generally under water-table (unconfined) conditions. Artesian (confined) conditions predominate in most other parts of groundwater reservoirs of Long Island.
>
> There are several distinctive features about Long Island which affect its hydrogeological behavior and hence influence how solutes such as aldicarb may move. First, both the Pleistocene upper glacial material, in which the water-table aquifer is developed and on which are the island soils, and the deeper, dominantly artesian, Cretaceous Magothy aquifer are mainly unreactive quartz (SiO_2) grains with little clay or organic material and an almost total absence of carbonate minerals. Because of an absence of reactive minerals, the chemistry of groundwater tends to be like that of recharging rainfall--slightly acid, pH 5-6, with low salt content. Further, the scarcity of reactive clay minerals and organic material tends to limit the sorbtive capacity of the aquifers.

The glacial and Magothy materials, in addition to their lack of chemical reactivity, have an above-average ability to transmit water. Thus, rainfall on the island tends to percolate readily through the soil to the zone of saturation where it moves laterally as groundwater to discharge to the ocean or to streams and inlets along the shore. Because of this ability of Long Island soils to accept rainfall and transmit it directly downward, little rainfall runs off the surface of the soil, and thus there is little development of streams on the island.

The site selected for the modeling of pesticide transport on a local scale was the Wickham farm. The study field is located on the south shore of the North Fork of Long Island near the town of Cutchogue. According to the data supplied INTERA by the EPA, the field comprises approximately 6.5 acres, and was subjected to three biannual aldicarb applications, as indicated in Table 6-1. This site was chosen from a number of possible alternatives for the following reasons:

1. No source of aldicarb exists up the hydraulic gradient from this field. Thus, all aldicarb found in groundwater under and downgradient from the field must be from aldicarb applied to the field.

2. The depth of the water table under the field is shallow enough that wells for sample collection could be installed and samples of the unsaturated soil down to the water table taken with minimal difficulty.

3. The amounts and dates of aldicarb application to the field were known.

4. The hydrogeological conditions and aldicarb application rates are representative of those on the Island.

Table 6-1. ALDICARB APPLICATION RATES - WICKHAM FARM

Date*	Nominal Aldicarb Mass Applied (lbs active ingredient/acre)
April 15, 1977	2.0
June 10, 1977	1.2
April 15, 1978	2.25
June 20, 1978	1.8
April 15, 1979	2.85
June 10, 1979	2.25

* Actual application dates may have varied ± one week, depending on the stage of growth of the crop.

A map of the Wickham field site is shown in Figure 6.1 and an idealized longitudinal cross-section is shown in Figure 6.2.

6.2 THE PESTICIDE ALDICARB

Aldicarb is a nematicide, acaricide, and a systemic insecticide. Its environmental fate is dominated by two factors: the fact that it forms two toxic daughter products, and its high mobility in soils. Degradation of the toxic residues of the compound is of intermediate duration compared to other pesticides.

Aldicarb is a white crystalline solid which is incorporated into soil as a granule containing either 10% or 15% active ingredient. In order to be effective, it must dissolve in water. Once this happens in soils, the compound begins to transform and degrade.

The current theory is that aldicarb, 2-methyl-2-(methylthio)propionaldehyde O-(methylcarbamoyl)oxime, is fairly rapidly oxidized to aldicarb sulfoxide, 2-methyl-2-(methylsulfinyl)propionaldehyde O-(methylcarbamoyl) oxime, which in turn is more slowly oxidized to aldicarb sulfone, 2-methyl-2-(methylsulfonyl)propionaldehyde O-(methylcarbamoyl)oxime. Concurrently, these three carbamates are transformed by hydrolysis to corresponding oximes. Hydrolysis is a chemical reaction in which water breaks up an organic molecule (RX), such as aldicarb, by breaking a carbon-X bond and replacing it with OH from the water molecule:

$$R\text{-}X + H_2 \rightarrow R\text{-}OH + X^- + H^+ \qquad (6\text{-}1)$$

These products of hydrolysis are far less toxic than aldicarb, its sulfoxide or its sulfone, and are of little environmental concern (Smelt et al. 1978). A schematic of these processes is shown in Figure 6.3.

Recently, Dean et al. (1988) performed a detailed review of degradation and transformation rates and adsorption coefficients for aldicarb and its two daughter products.

6.3 EXAMPLE PROBLEMS

Two example model applications are discussed in this section. The first, P2S, is a PRZM to SAFTMOD linkage. The second, P2V, is a PRZM/VADOFT/SAFTMOD linkage.

6.3.1 Example Problem One - PRZM To SAFTMOD Linkage (P2S)

In the first example problem, PRZM and SAFTMOD are linked directly, without using VADOFT. SAFTMOD is used in the X-Z mode. It was assumed that aldicarb flux, but no recharge water, enters the aquifer. A problem of this type is probably the simplest which can be addressed with the linked model.

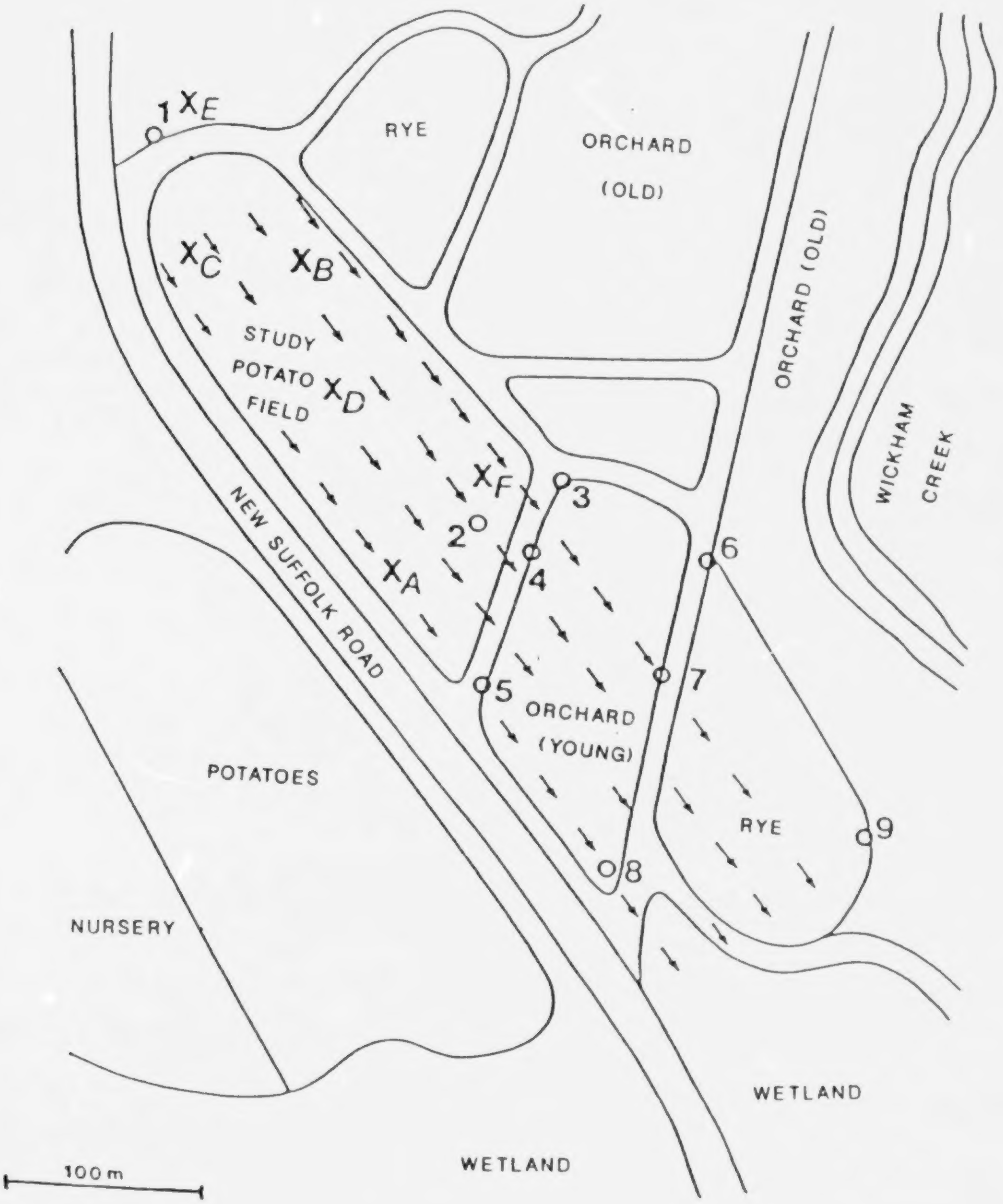

1
XE
RYE
ORCHARD
(OLD)
ORCHARD (OLD)
XC
XB
STUDY
POTATO
FIELD
XD
XF
3
2
4
XA
6
WICKHAM
CREEK
NEW SUFFOLK ROAD
5
7
ORCHARD
(YOUNG)
POTATOES
RYE
9
8
NURSERY
WETLAND
WETLAND
100 m

Figure 6.1. Map of the Wickham Field study site.

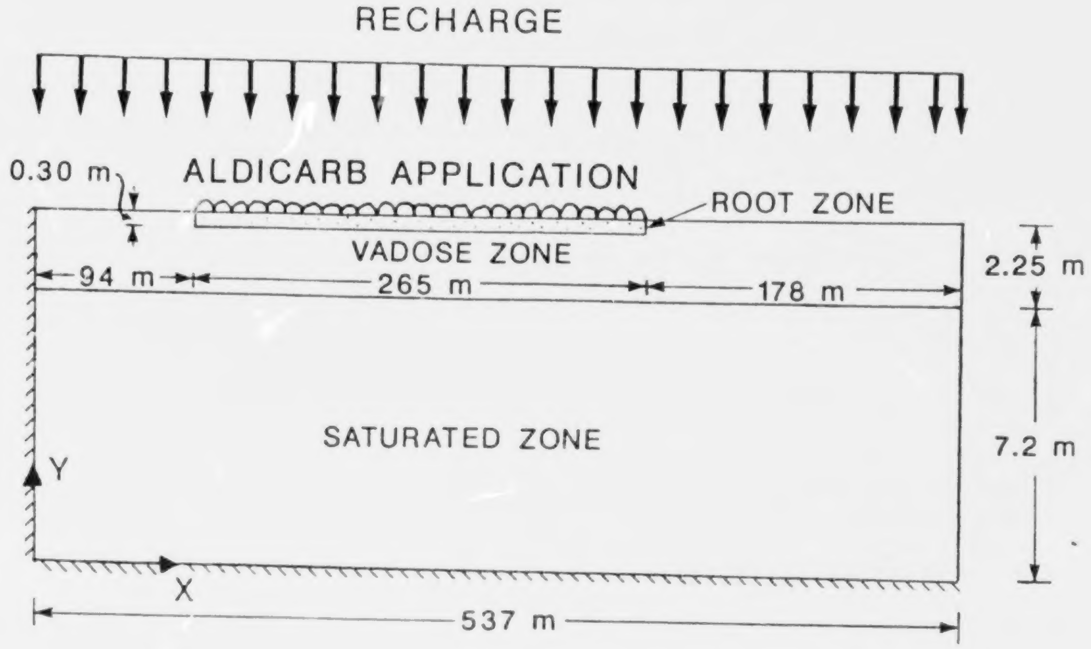
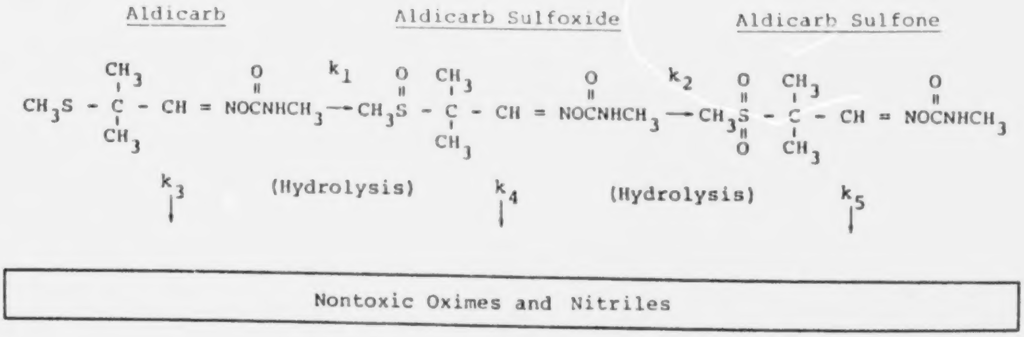

RECHARGE
0.30 m
ALDICARB APPLICATION
ROOT ZONE
VADOSE ZONE
94 m
265 m
178 m
2.25 m
SATURATED ZONE
7.2 m
Y
X
537 m

Figure 6.2. Longitudinal cross-section of Wickham Field study site.



$$CH_3S-\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}-CH=NO\overset{\overset{O}{\|}}{C}NHCH_3 \xrightarrow{k_1} CH_3\overset{\overset{O}{\|}}{S}-\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}-CH=NO\overset{\overset{O}{\|}}{C}NHCH_3 \xrightarrow{k_2} CH_3\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}-CH=NO\overset{\overset{O}{\|}}{C}NHCH_3$$

Aldicarb
Aldicarb Sulfoxide
Aldicarb Sulfone
k1
k2
k3
(Hydrolysis)
k4
(Hydrolysis)
k5
Nontoxic Oximes and Nitriles

Figure 6.3. Schematic of aldicarb environmental chemical pathways.

Specifics of the model input sequences are described below, followed by simulation results and comparison to observed data.

6.3.1.1 PRZM Input--
PRZM was used to simulate the crop root zone, the upper 60 cm of the profile. The PRZM input data set is shown in Figure 6.4. Pertinent features of the input are discussed below.

Uptake of the pesticide was simulated (UPTKF=1.0). Soil temperature was simulated (ITFLAG=1) with a bottom boundary temperature of 26°C. Values of thermal conductivity and heat capacity were estimated by the model (IDFLAG=1). For the purpose of calculating soil thermal properties, the sand, clay, and organic carbon percentage of each horizon was assumed to be 60, 30, and 2, respectively. Volatilization was also simulated. The diffusion coefficient for the chemical in air was set to 4300 cm^2 day^{-1}. A Henry's Law Constant (cm^3 cm^{-3}) of 1.7 x 10^{-7} was used. No temperature correction was made for the Henry's Law Constant (ENPY = 0.0). Monthly values of albedo (ALBEDO) for the temperature simulation were set to 0.15, the emissivity of the soil set to 0.97, and the measurement height of the wind speed in the meteorological file was assumed to be 2 meters.

Three soil horizons were utilized. The first was 30 cm in thickness, with 5-cm layer thicknesses (DPN). Bulk density (BD) in the layer was 1.38 g cm^{-3}, and the field capacity and wilting point water contents (THEFC and THEWP) were set to 0.24 and 0.10 cm^3 cm^{-3}, respectively.

The chemical partition coefficient was set at 0.20 cm^3 g^{-1} and the decay rate was set to 0.0035 day^{-1}.

In the second horizon (total thickness of 30 cm), layer thickness was greater (10 cm), bulk density slightly higher (1.59 g cm^{-3}), and field capacity and wilting point water contents lower (0.042 and 0.02, respectively). The partition coefficient was set to 0.20 cm^3 g^{-1} and the decay rate was 0.0035 day^{-1}.

The third horizon (885 cm) was similar to the second, with layer thicknesses of 8.85 cm, slightly lower THEFC (0.035), THEWP (0.015), and partition coefficient (0.16). The decay rate was set to 0.00076 day^{-1}. The user should note that a total of 115 soil layers were used to simulate the PRZM domain from the soil surface to the base of the aquifer.

6.3.2 SAFTMOD Input

6.3.2.1 Flow--
For the SAFTMOD flow simulation, 451 nodes (400 elements) were used in an X-Z configuration with no recharge. Nodal spacing was 13.125 meters in the 'x' direction and 0.72 m in the 'z' direction. The aquifer was assumed to be approximately 7.2 m thick, with a constant gradient of 0.00074 m m^{-1}. This results from the use of constant head conditions at the upstream and downstream boundaries of 7.6 m and 7.2 m, respectively. The hydraulic conductivity in the 'x' direction was taken to be 100 m day^{-1} and in the 'z' direction, 10 m day^{-1}. The specific storage of the aquifer material was

```
PRZM W/ DAUGHTER PRODUCTS FOR ALDICARB
HYDOLOGY PARAMETERS FOR WICKHAM FIELD SITE
    .780    .000       1  30.000       1       3
    10.1    10.0    12.4    13.3    14.9    15.0
    15.2    14.2    12.5    11.5    10.0     9.7

       0
       1
       1    .150    60.0  75.000       3  20  20  20 0.3 0.3 0.3    60.0
       3
  150477  150977  300977       1
  150478  150978  300978       1
  150479  150979  300979       1
ALDICARB TRANSPORT AND TRANSFORMATION AND APPLICATION PARAMETERS
       6       1
ALDICARB
  150477    10.0    2.24
  100677    10.0    1.35
  140478    10.0    2.52
  100678    10.0    2.02
  150479    10.0    3.19
  100679    10.0    2.52
       1       1
SOILS PARAMETERS FOR WICKHAM FIELD SITE
   945.0     1.0   0   0   0   0   0   0   1   1
   4.3E3  1.7E-7          5.5E-3          5.0E-3
 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.97  2.0
 26.0 26.0 26.0 26.0 26.0 26.0 26.0 26.0 26.0 26.0 26.0 26.0
       3
       1    30.0    1.38   0.055                 0.0   .0035   0.003   0.003
             5.0    .240    .100                0.20
            26.0    60.0    30.0     2.0
       2    30.0    1.59   0.042                 0.0   .0035   0.003   0.003
            10.0    .042    .020                0.20
            26.0    60.0    30.0     2.0
       3   885.0    1.59   0.035                 0.0  7.6E-4   0.003   0.003
            8.85    .035    .015                0.16
            26.0    60.0    30.0     2.0
       0       0
    WATR    YEAR       1    PEST    YEAR       1    CONC    YEAR       1
       2
    INFL    TSER      15     1.0
    AFLX    TSER      15     1.0
```

Figure 6.4. PRZM input data set - PRZM to SAFTMOD linkage.

taken to be 1.0×10^{-5} m^{-1}; the specific yield, 0.24. The SAFTMOD flow input data set is shown in Figure 6.5. Specific values of key parameters for flow and transport are summarized in Table 6-2.

Table 6-2. KEY PARAMETER VALUES USED IN THE SIMULATION OF GROUNDWATER FLOW AND PESTICIDE TRANSPORT IN THE SATURATED ZONE (EXAMPLE NUMBER 1)

Parameter	Coarse Sand	Units
Saturated hydraulic conductivity, K_x	100	$m\ d^{-1}$
Saturated hydraulic conductivity, K_z	10	$m\ d^{-1}$
Porosity, ϕ	0.3	——
Specific yield, S_y	0.24	——
Specific storage, S_s	10^{-5}	m^{-1}
Longitudinal dispersivity, α_L	10	m
Vertical dispersivity, α_T	0.2	m
Retardation factor, R	1.86	——
Decay coefficient, γ	7.6×10^{-4}	d^{-1}

6.3.2.2 Transport--

For transport, the same grid spacing was used as for flow. An effective porosity of 0.3 $m^3\ m^{-3}$ was used along with a retardation factor of 1.86 and a degradation constant of 0.00076 day^{-1}. A dispersivity of 10 m in the 'x direction and 0.2 m in the 'z' direction was used. The SAFTMOD transport input data set is shown in Figure 6.6.

6.3.3 Example Problem Two - PRZM/VADOFT/SAFTMOD Linkage (P2V)

The second example problem involves the use of all three models. The simulation conditions were essentially the same except that VADOFT was used to simulate the lower portion of the vadose zone. The PRZM input file (Figure 6.7) was modified so that it would simulate only the top of the vadose zone.

The VADOFT flow and transport input sequences are discussed below.

```
***************************************************************
***                  SAFTMOD  FLOW
***************************************************************
***Group1
LONG ISLAND ALDICARB : X-Z FLOW WITH NO RECHARGE
***Group2
    1    0    0    1    0    1    0    0
***Group3
    1    1    1    1  451  400    1    1
***Group4
    1   10     0.010
***Group5
    1    1    0    1    1    0    0    0    0    0    0
***Group7
   11   41    0    0    0
    13.125      0.72       1.0       1.0    13.125      0.72     525.0       7.2
***Group8
    1    1    1
    1    1    1  400    1    1
***Group9
     1500.      150.    1.E-05       .24     0.000
***Group14
    1   22
   55   66   77   88   99  110  121  132  143  154  165  176  187  198  209  220
  231  242  253  264  275  286
***Group15
   22    0    0    0
***Group16
    1      7.60
    2      7.60
    3      7.60
    4      7.60
    5      7.60
    6      7.60
    7      7.60
    8      7.60
    9      7.60
   10      7.60
   11      7.60
  441        7.2
  442        7.2
  443        7.2
  444        7.2
  445        7.2
  446        7.2
  447        7.2
  448        7.2
  449        7.2
  450        7.2
  451        7.2
***Group20
    7.2
    0    0    0
***Group22
   11
  441  442  443  444  445  446  447  448  449  450  451
```

Figure 6.5. SAFTMOD flow input data set.

```
***************************************************************
***                 SAFTMOD TRANSPORT
***************************************************************
***Group1
LONG ISLAND ALDICARB : X-Z TRANSPORT WITH NO RECHARGE
***Group2
    0    0    0    1    0    0    0    0
***Group3
    1    1    1    1  451  400    1    1
***Group4
    1    1      0.01
***Group5
    1    1    0    1    0    0    1    0    1    0    0
***Group7
   11   41    0    0    0
    13.125      0.72       1.0       1.0    13.125      0.72      525.0       7.2
***Group8
    1    1    1
    1    1    1  400    1    1
***Group9
      10.0      0.2          0        0.3       0.0
***Group13
    0
      1.86   0.0114       0.0
***Group14
    1   22
   55   66   77   88   99  110  121  132  143  154  165  176  187  198  209  220
  231  242  253  264  275  286
***Group15
   11    0    0    0
    1       0.0
    2       0.0
    3       0.0
    4       0.0
    5       0.0
    6       0.0
    7       0.0
    8       0.0
    9       0.0
   10       0.0
   11       0.0
***Group20
       0.0
    0    0    0
***Group22
   11
  441  442  443  444  445  446  447  448  449  450  451
***Group24
   19
  255  265  266  277  288  289  299  313  324  325  335  363  374  375  385  423
  434  435  445
```

Figure 6.6. SAFTMOD transport input data set.

```
PRZM W/ DAUGHTER PRODUCTS FOR ALDICARB
HYDOLOGY PARAMETERS FOR WICKHAM FIELD SITE
    .780    .000       1  30.000       1       3
    10.1    10.0    12.4    13.3    14.9    15.0
    15.2    14.2    12.5    11.5    10.0     9.7

       0
       1
       1    .150    60.0  75.000       3   20   20   20 0.3 0.3 0.3    200.0
       3
  150477  150977  300977       1
  150478  150978  300978       1
  150479  150979  300979       1
ALDICARB TRANSPORT AND TRANSFORMATION AND APPLICATION PARAMETERS
       6       1
ALDICARB
  150477    10.0    2.24
  100677    10.0    1.35
  140478    10.0    2.52
  100678    10.0    2.02
  150479    10.0    3.19
  100679    10.0    2.52
       1       1
SOILS PARAMETERS FOR WICKHAM FIELD SITE
    60.0     1.0   0   0   0   0   0   0   1   1
   4.3E3  1.7E-7          5.5E-3          5.0E-3
 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.97  2.0
 26.0 26.0 26.0 26.0 26.0 26.0 26.0 26.0 26.0 26.0 26.0 26.0
       2
       1    30.0    1.38   0.055             0.0   .0035   0.003   0.003
             5.0    .240    .100            0.20
            26.0    60.0    30.0     2.0
       2    30.0    1.59   0.042             0.0   .0035   0.003   0.003
            10.0    .042    .020            0.20
            26.0    60.0    30.0     2.0
       0       0
    WATR    YEAR       1    PEST    YEAR       1    CONC    YEAR       1
       2
    INFL    TSER      15     1.0
    AFLX    TSER      15     1.0
```

Figure 6.7. PRZM input data set - PRZM to VADOFT link.

6.3.3.1 VADOFT Flow--

The VADOFT flow input sequence is shown in Figure 6.8. For the PRZM/VADOFT/SAFTMOD linkage, the vadose zone was divided into three layers. Layer 1 is 90 cm thick and discretized into 12 linear elements, layer 2 is 75 cm thick with 8 elements while layer 3 is 720 cm thick with 72 elements. Although Figure 6.8 shows that two soil materials were assigned to the vadose zone, the material properties were assumed homogeneous. The saturated hydraulic conductivity was taken to be 432 cm day^{-1}. The effective porosity was estimated to be 0.3 cm^3 cm^{-3}, the specific storage of the material 0.0, and the air entry pressure head 0.0 cm. The closed-form solution embedded in the codes for generating soil water characteristic curves was used. The coefficient values used were $n = -0.1$, $\alpha = 0.124$, $\beta = 2.28$, and $\gamma = 0.56$. Residual water-phase saturation was taken to be 0.14 cm^3 cm^{-3}. Table 6-3 is a summary of the key parameters for vadoze zone flow and transport.

Table 6-3. PARAMETER VALUES USED IN THE SIMULATION OF INFILTRATION AND PESTICIDE TRANSPORT IN THE VADOSE ZONE (VADOFT SIMULATIONS)

Parameter	Loamy Sand	Units
Saturated hydraulic conductivity, K_{sat}	432cm	d^{-1}
Porosity, ϕ	0.4	——
Residual water saturation, S_{wr}	0.14	——
Air entry value, ψ_a	0.0	——
Moisture retention parameter, α	0.124	cm^{-1}
Moisture retention parameter, β	2.28	——
Moisture retention parameter, γ	0.56	——
Dispersivity, α_L	4.0	cm
Retardation factor, R	1.86	——
Decay coefficient, λ	0.00076	d^{-1}

Flow boundary conditions are prescribed for VADOFT at the upper boundary and head boundary conditions are prescribed at the lower end. The head boundary value is based on SAFTMOD-predicted water level elevation.

```
***************************************************************
***                    VADOFT FLOW
***************************************************************
***group1
LONG ISLAND ALDICARB APPLICATION: VADOSE ZONE FLOW SIMULATION
***group2
   93   30    2    1    1    1    1    1    1    0    0
   10    2    1       .01
***group3
    1    1    1   30    1    1    0    0
***group4
       0.0       1.0       1.0       1.0
   15    1     -0.01       1.0
***group5
    3
    1   12    1      90.0
    2    8    2      75.0
    3   72    2     720.0
***group6
     720.0    0
***group7
    0    1       0.0     720.0    1    0
***group8
   4.32E02    0.3E00    0.0E00    0.0E00
   4.32E02    0.3E00    0.0E00    0.0E00
***group9
  0.140E00   -1.0E00 0.124E00   2.28E00   0.56E00
  0.140E00   -1.0E00 0.124E00   2.28E00   0.56E00
```

Figure 6.8. VADOFT flow input data set.

```
***************************************************************
***                    VADOFT TRANSPORT
***************************************************************
***group1
TRANSPORT SIMULATION -- 1 CHEMICAL - 5 MONTHS
***group2
   93   30    3    0    1    0    1    1         0    1
***group3
    0    1    1    1    0    1    0    0
***group4
       0.0       1.0       1.0       1.0
   15    1     -0.01       1.0
***group5
    3
    1   12    1      90.0
    2    8    2      75.0
    3   72    3     720.0
***group6
       0.0    0       0.0    0       0.0    0
***group7
    0    0       0.0       0.0    1    0
***group8
   4.00E00    0.3E00   1.86E00    0.0E00   1.61E00    0.0E00   1.61E00    0.0E00
   4.00E00    0.3E00   1.86E00    0.0E00   1.61E00    0.0E00   1.61E00    0.0E00
      10.0       0.3      1.86       0.0      1.86       0.0      1.86       0.0
***group11
*** MATERIAL 1
    1       0.0       1.0    0.5E00         0
    1    7.6E-4       0.0    5.0E-3     0.984    5.0E-3     0.984
*** MATERIAL 2
    2       0.0       1.0    0.5E00         0
    2    7.6E-4       0.0    5.0E-3     0.984    5.0E-3     0.984
*** MATERIAL 3
    3       0.0       1.0    0.5E00         0
    3    7.6E-4       0.0    7.6E-3     0.984    7.6E-3     0.984
***group12
    1    0
***group15
   21   31
```

Figure 6.9. VADOFT transport input data set.

6.3.3.2 VADOFT Transport--

For transport, the same grid spacing was used. The VADOFT transport input sequence is shown in Figure 6.9. Three soil materials were assigned to the vadose zone. Effective porosity, retardation and decay rate were assumed uniform for each material with values of 0.3, 1.86 and 7.6×10^{-4} day^{-1}, respectively. Dispersivity was assumed to be the same for materials 1 and 2 with a value of 4 cm while a dispersivity of 10 cm was assumed for material 3.

VADOFT transport boundary conditions are prescribed when run in the linked mode. At the upper boundary, a prescribed flux is utilized, the value of which is determined by PRZM solute flux output. At the lower boundary, a zero-concentration condition is utilized.

6.3.4 Simulation Results

The simulation was run for three years using meteorological data provided by EPA (Bob Carsel, personal communication). For the most part, initial parameter values were taken from Lafleur et al. (1981) and were adjusted through the calibration process to achieve results which correlated as well as possible with the observed data. Data taken during December 1979 for the vadose zone and the saturated zone were utilized for comparison to simulation results.

6.3.4.1 Vadose Zone Results--

Observed and simulated concentration profiles using PRZM (P2S simulation) and VADOFT (P2V simulation) are shown in Figure 6.10. Note that the observed data are shown for three of the five cores having concentrations reported by Lafleur et al. (1981). The two remaining cores contained almost no residues and were not plotted. Simulated peak concentrations were on the order of 175 mg kg^{-1} and occurred at a depth of approximately 100 cm below land surface, whereas the observed concentrations were much lower, with the peak occurring at approximately 75 cm below land surface (the peak concentration observed was 118 mg kg^{-1}). With the parameters selected for these simulations, groundwater concentrations of sufficient magnitude to match the observed values could not be simulated without this magnitude of concentrations in the vadose zone. With the selected parameters, both PRZM and VADOFT simulate movement of the peak further into the profile than the observed data. However, it should be noted that earlier calibration work by Carsel et al. (1985), with PRZM I, by Donigian (personal communication, 1989) with PRZM II, and by Huyakorn et al. (1988) with VADOFT, demonstrated much better agreement between observed and simulated vadose zone concentrations using a decay rate of 0.002 day^{-1} (instead of 0.00076 day^{-1}) for the vadose region between the root zone and the water table. The results presented here are only for demonstration of the linked operation of RUSTIC.

6.3.4.2 Saturated Zone Results--

Figure 6.11 shows simulated aldicarb concentrations in an X-Z cross section of the modeled area in December 1979 for P2S linkage and Figure 6.12 show the same for the P2V linkage. Note that the concentrations are skewed to the right, indicating the influence of the regional gradient. Figure 6.13 shows the simulated versus observed concentrations with depth for Wells W-2, -4, -5, and -7. Note the position of these wells from Figure 6.1. The simulationof concentrations in Wells W-2 and W-4, which are essentially in the field, are excellent with the exception of the shallowest depth (0.8 m below the water table) in Well W-2. Observed concentrations at Wells W-5 and W-7, which are further downgradient, are less well matched by the simulation results. In these wells, the shallowest observations are better simulated than the deeper observations.

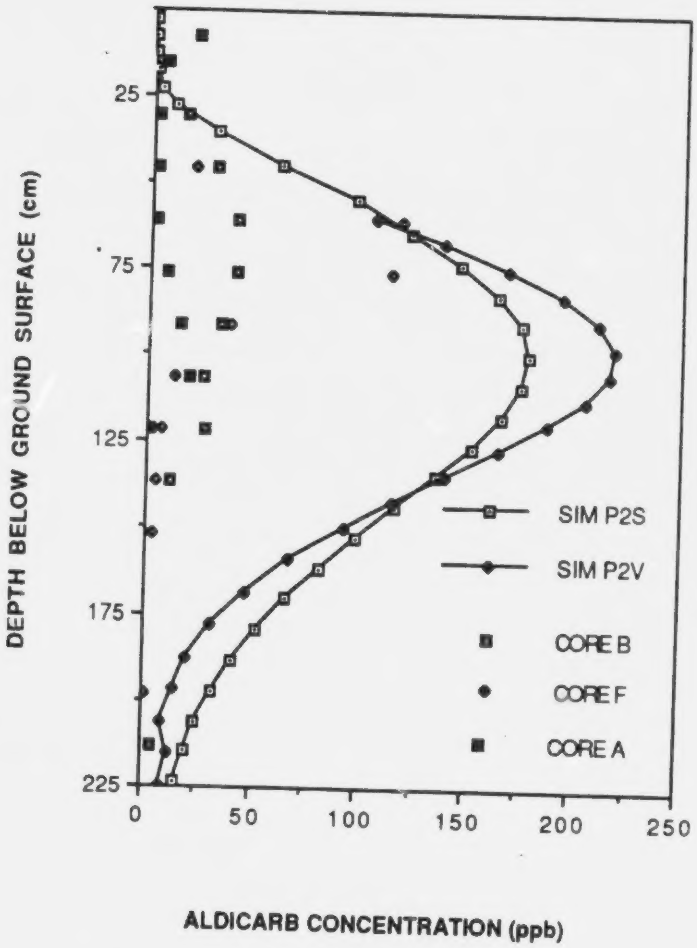


Figure 6.10. Observed and simulated aldicarb distribution in the vadose zone, December 1979.

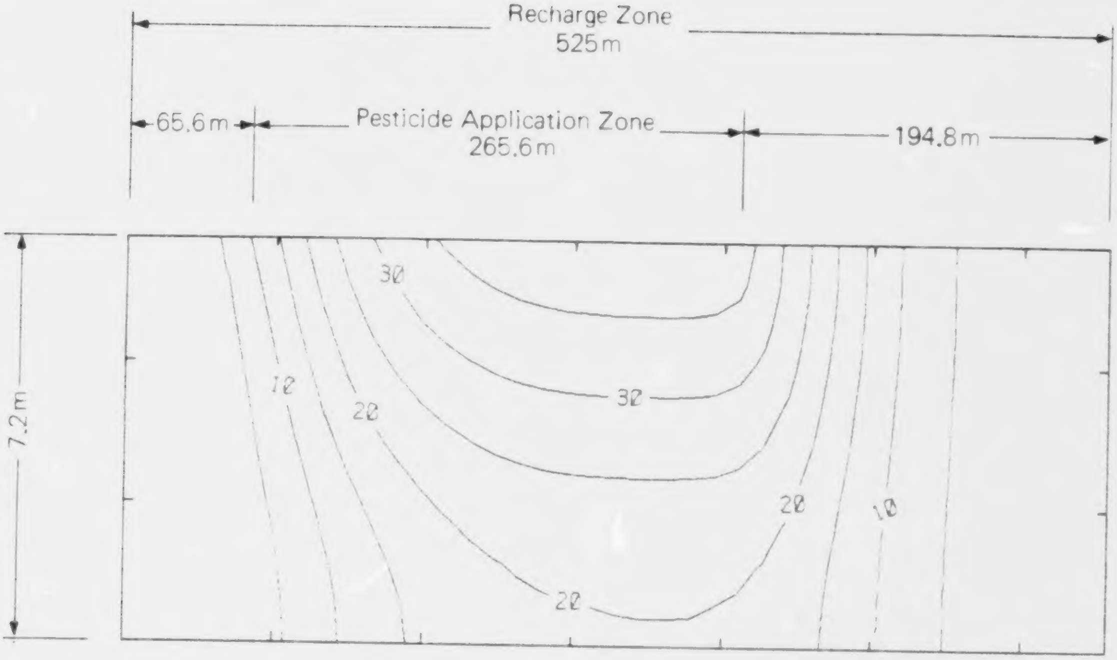


Figure 6.11. Simulated aldicarb concentrations in the saturated zone, December 1979 (P2S).

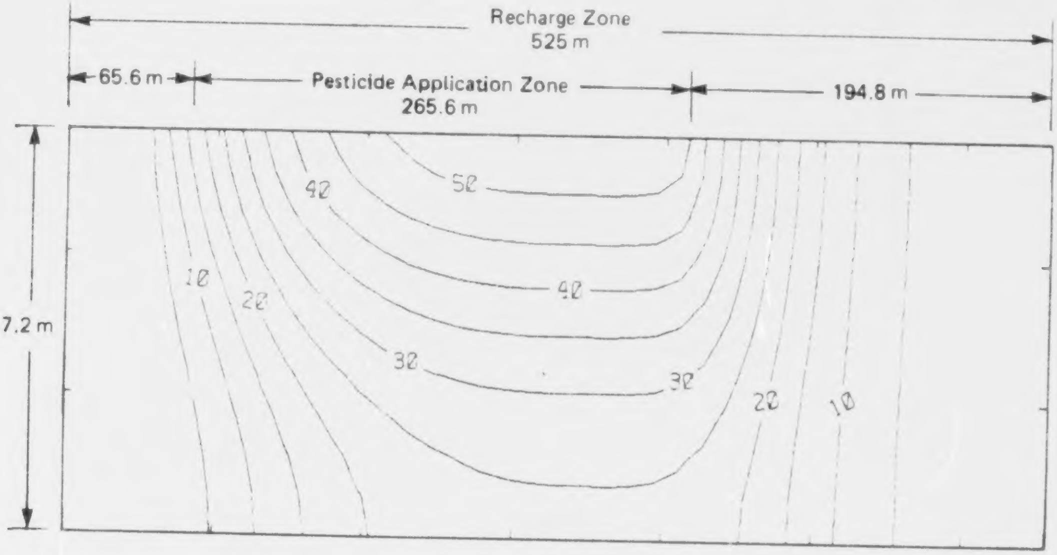


Figure 6.12. Simulated aldicarb concentrations in the saturated zone, December 1979 (P2V).

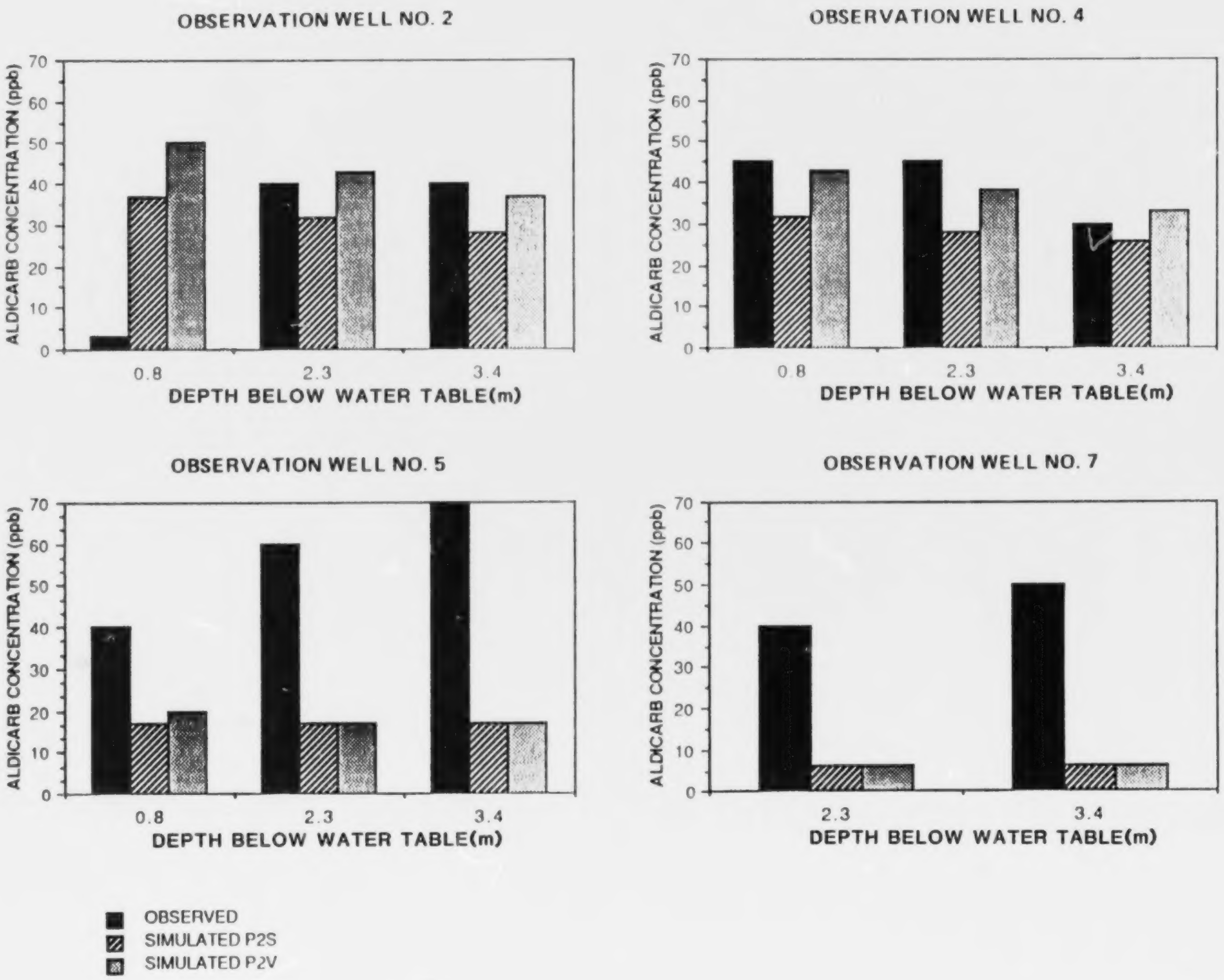


Figure 6.13. Comparison of observed and simulated concentrations in the saturated zone, December, 1979.

SECTION 7

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SECTION 8

APPENDICES

8.1 ERROR MESSAGES AND WARNINGS

The RUSTIC Code contains a number of error and warning messages which indicate either fatal or non-fatal routine conditions. A list of the current error (fatal) and warning (non-fatal) conditions which are recognized by the code is given in Table 8-1. Along with each message, troubleshooting approaches are described. Error or warning messages originating in RUSTIC (the main code) are numbered beginning with 1000; PRZM, 2000; VADOFT, 3000; SAFTMOD, 4000; and the Monte Carlo module, 5000. Note that error numbers less than 1000 may appear. These numbers are being supplied by the FORTRAN compiler which was used to compile RUSTIC and its associated modules. These errors will probably be associated with reading input data; e.g., problems such as inappropriate characters in an input field which the code is attempting to interpret as an integer or a disk drive being unavailable for reading data. Consult the compiler errors list for the exact cause.

Note also that if the compiler used uses numbers in the range of 1000 to 5000 for these file access errors an error number may appear which seems to be an EXESUP/PRZM/VADOFT/SAFTMOD error. The error message will not, however, correspond to the messages in Table 8-1. The message will be something such as: "Error in attempting to open file [<file name>]" or "Error in input...." Again, check the compiler's run time error list for the exact cause.

When errors and warnings are reported in the output echo file, three lines of information are provided. The first line reports the number and whether the condition was an error (fatal) or warning (non-fatal). The second line supplies the associated message. The third line supplies the subroutine trace of where the error occurred. For example, the third line might be: 'RUSTIC>INPREA>VADINP'. This implies that the error occurred in the subroutine VADINP (the VADOFT input routine), which was called from subroutine INPREA, which was called from the RUSTIC main program. This third line will not appear if an error occurs in the routine INITEM, which is the routine to read the RUSTIC.RUN file and initialize the simulation.

8.2 VARIABLE GLOSSARY

This section presents the major variables used in the RUSTIC code. Table 8-2 presents variables used in the EXESUP module, Table 8-3 presents PRZM variables, Table 8-4 presents VADOFT variables, Table 8-5 presents SAFTMOD variables and Table 8-6 presents variables used in the Monte Carlo module.

Table 8-1. RUSTIC ERROR MESSAGES, WARNINGS, AND TROUBLESHOOTING APPROACHES

	Error or Warning	Troubleshooting Approach/Explanation
1000	nnn negative water fluxes into SAFTMOD zone nn	Negative values of water flux have been set to zero in WMFCAL. This is normal. No action necessary.
1010	Water table is above vadose zone	The water table has accumulated to above the top of the vadose zone. Use higher conductivities in SAFTMOD or increase the thickness of the vadose zone.
1020	Water table is above root zone	The water table is above the top of the root zone. Use higher conductivities in SAFTMOD or increase the thickness of the root zone.
1040	Zero aquifer thickness in MASCOR	Check the values used to define the SAFTMOD grid in the SAFTMOD input data.
1050	Zero or negative mass in VADOFT/PRZM nodes below the water table	This is a warning only, the concentration values in the VADOFT or PRZM nodes below the water table will not be adjusted for the current timestep by what mass was simulated within the SAFTMOD common volume. If this warning appears repeatedly, the VADOFT or PRZM and SAFTMOD geometry might have to be adjusted.
1060	VADOFT and SAFTMOD were selected w/o PRZM	If VADOFT and SAFTMOD are run in linked mode, PRZM must also be utilized. Turn PRZM "ON" in global parameter file and provide a PRZM input parameter file.
1070	Error in the file name input, line with...	An incorrect (or misspelled) identifier was supplied for a file (ANAME of group EXESUP2, see Section 4.2.1.2).
1080	Value of NLDLT [nnnn] exceeds MXVDT [nnnn]	The number of PRZM/VADOFT timesteps specified exceeds the maximum number in the PARAMETER statement. Reduce the number of timesteps or increase the maximum number in the PARAMETER statement. If the latter, recompile the code.
1082	Value of NLDLT [nnnn] is less than 1	NLDLT must be greater than 0 in the global data group of RUSTIC input.

Table 8-1. RUSTIC ERROR MESSAGES, WARNINGS, AND TROUBLESHOOTING APPROACHES (continued)

	Error or Warning	Troubleshooting Approach/Explanation
1084	NLDLT [nnnn] has been reset to the calculated total number of days [nnn]	The value of NLDLT which was input was greater than the total number of days calculated from the starting and ending dates. This is a warning only, but to avoid it, set NLDLT to be less than or equal to the total number of days between the start and end of simulation.
1090	Bad value [nnnn] for number of chemicals	The number of chemicals must be between 1 and 3, inclusive. Change the number in the global data group of RUSTIC input file.
1092	Bad index [nnnn] of chemical	An invalid index was provided for input record EXESUP3 with ANAME = 'PARENT OF'. Values less than 1 or greater than NCHEM are not valid.
1100	Bad value [nnnn] for chemical parent species	Check input values. Chemical 1 can have a a parent of 0 only. Chemical 2 can have a parent of 0 or 1. Chemical 3 can have a parent of 0, 1, or 2.
1190	Bad identifier reading global data [<value>]	An invalid label appears in the global data section (EXESUP) of the RUSTIC.RUN input file.
1200	End date is before start date	Check the 'START DATE' and 'END DATE' records of RUSTIC.RUN input file.
1202	End date and start date are the same	Check the 'START DATE' and 'END DATE' records of RUSTIC.RUN input file.
1210	Unrecognized label [<label>] while attempting to read ECHO or TRACE	A record in the RUSTIC.RUN file appears after the 'ENDDATA' record before the 'ECHO' or 'TRACE' records.'
1220	Echo level not defined; set to 5 [or 1]	No output echo level was specified in the global parameter file. The value was set to 5 if MONTE CARLO was not selected or 1 if MONTE CARLO was selected.
1230	Trace level not defined; set to 0	No subroutine trace level was specified in the global parameter file. The value was set to the default value of 0.

Table 8-1. RUSTIC ERROR MESSAGES, WARNINGS, AND TROUBLESHOOTING APPROACHES (continued)

	Error or Warning	Troubleshooting Approach/Explanation
1240	End of file on RUSTIC run file	Recheck the global data group of the RUSTIC input file. There is an error in the input sequence; an option was set which required more lines of data than supplied.
1250	Error reading RUSTIC run file data...	Error in reading RUSTIC input data, most likely there are inappropriate characters in a data field which is attempting to be interpreted as integer data.
1270	Too many files requested to be open at once	The maximum number of files allowed (defined in the include file IOUNITS.PAR) is too small a number for the (recently modified) version of RUSTIC. This error should not appear in the current version of RUSTIC.
1280	ENDFILE statement present before file [nn] was opened	An input file, which is required for the current RUSTIC simulation configuration, has not been identified in the file group of the RUSTIC input file.
1290	Request to close file [nn] which was not open	Should never occur in current version of RUSTIC. Implies that recent code modifications have been made which did not properly account for which files were open.
1300	Unknown unit number to open file	Should never occur in current version of RUSTIC. Implies that recent code modifications have been made which did not properly account for which files were open.
1310	Too many lines required for Trace Option	Should never occur in current version of RUSTIC. Implies that recent code modifications have been made resulting in a very high level of subroutine nesting.
1320	Argument [<value>] too large for EXP	Attempt to take the exponential of too large a real number.
1330	Negative or zero argument [<value>] to LOG	Attempt to take the log of a zero or negative argument.

Table 8-1. RUSTIC ERROR MESSAGES, WARNINGS, AND TROUBLESHOOTING APPROACHES (continued)

	Error or Warning	Troubleshooting Approach/Explanation
1350	Single precision overflow	A mathematical operation resulted in a number too large for the real value being calculated.
1360	Negative argument [<value>] to SQRT	Attempt to take the square root of a negative number. Subroutine trace accompanying error message will show in which routine the error occurred.
1390	Invalid index [nnnn] in reading record [<record number>]	A bad index value in a VADOFT or SAFTMOD read, probably initial condition data.
1400	Error reading PRZM data	Probable causes are inappropriate characters in an input field for integer or real reads.
1500	ENDDATA before starting day was provided	The label 'ENDDATA' appears in the global parameters section of RUSTIC.RUN file before the 'START DATE' record was provided.
1510	ENDDATA before end day was provided	The label 'ENDDATA' appears in the global parameters section of RUSTIC.RUN file before the 'END DATE' record was provided.
1520	ENDDATA before time step was provided	The label 'ENDDATA' appears in the global parameters section of RUSTIC.RUN file before the 'TIME STEP' record was provided. The 'TIME STEP' record is required if SAFTMOD is on.
1530	ENDDATA before number of chemicals was provided	The label 'ENDDATA' appears in the global parameters section of RUSTIC.RUN file (with TRNSIM = 'ON') before the 'NUMBER OF CHEMICALS' record was provided. The 'NUMBER OF CHEMICALS' record is required for a transport simulation.
1540	ENDDATA before the parent of chemical n was provided	The label 'ENDDATA' appears in the global parameters section of RUSTIC.RUN file (with TRNSIM = 'ON' and NUMBER OF CHEMICALS greater than 1) before the 'PARENT OF n' record was provided.

Table 8-1. RUSTIC ERROR MESSAGES, WARNINGS, AND TROUBLESHOOTING APPROACHES (continued)

	Error or Warning	Troubleshooting Approach/Explanation
1550	dd/mm/yy - Invalid START (or END) DATE	An invalid date has been entered in the global parameters section of the RUSTIC.RUN input file. Check to see if the month being specified had the number of days which is being implied (e.g., 31/02/88 is not valid).
1560	End of file [<file identifier>] encountered	The end of the file specified was reached while still attempting to read data.
1570	Monte Carlo simulation - Echo level reset to 1	If an echo level greater than 3 is requested with Monte Carlo on, the echo level will be reset to 1. No action required.
2000	Simulation date (dd/mm/yy), meteorological date (dd/mm/yy) do not match	The meteorological data file is not aligned with the simulation data. There is probably a missing record in the data file or the simulation start and end dates specified in RUSTIC.RUN do not correspond to the dates in the meteorological data file.
2005	WDMS file not supported in RUSTIC version of PRZM	This error should not occur in current version of RUSTIC. If it does appear, recent and probably inappropriate changes have been made to the code.
2010	Number of chemicals in PRZM [nn] <> number of chemicals in EXESUP [nn]	The value supplied to the PRZM input file for the number of chemicals being simulated does not agree with the number supplied to the RUSTIC input file.
2040	NPI [nnnn] + NEW [nnnn] is greater than NPII [nnnn] in subroutine MOC	Decrease the number of PRZM compartments or increase the parameter NPII. If the latter, recompile the code. This error only occurs if the MOC rather than backward difference transport solution technique is used.
2050	Solution for tridiagonal matrix not found, previous day's values used	If this message appears repeatedly, the PRZM problem definition geometry should be reevaluated.

Table 8-1. RUSTIC ERROR MESSAGES, WARNINGS, AND TROUBLESHOOTING APPROACHES (continued)

	Error or Warning	Troubleshooting Approach/Explanation
2060	NDC [nnnn] is greater than NC [nnnn]	Change PRZM problem definition geometry so that the input value of NDC is less than or equal to the parameter NC or change the value of NC and recompile.
2070	NCPDS [nnnn] is greater than NC [nnnn]	Change PRZM problem definition geometry so that the input value of NCPDS is less than or equal to the parameter NC or change the value of NC and recompile.
2080	NAPS [nnnn] is greater than NAPP [nnnn]	Change PRZM problem definition geometry so that the input value of NAPS is less than or equal to the parameter NAPP or change the value of NAPP and recompile.
2090	NHORIZ [nnnn] is greater than NCMPTS [nnnn]	Change PRZM problem definition geometry so that the input value of NHORIZ is less than or equal to the parameter NCMPTS or change the value of NCMPTS and recompile.
2100	NCOM2+1 [nnnn] is greater than NCMPTS [nnnn]	Change PRZM problem definition geometry so that the input value of NCOM2 is less than the parameter NCMPTS or change the value of NCMPTS and recompile.
2110	NPLOTS [nnnn] is greater than 7	Reduce the number of requested plots.
2120	Sum of horizon thicknesses exceeds depth	Change PRZM problem definition geometry so that the sum of horizon thickness is equal to the user supplied total depth.
2130	Soil profile description is incomplete, data available for xx.xx of xx.xx cm	Change PRZM problem definition file so that soil profile data are supplied for the entire defined depth.
2140	Calculated field capacity water content exceeds the saturation value	Either decrease the soil bulk density or adjust the parameters for calculating field capacity water content (if THFLAG=1) or lower the supplied value of field capacity water content (if THFLAG=0).

Table 8-1. RUSTIC ERROR MESSAGES, WARNINGS, AND TROUBLESHOOTING APPROACHES (continued)

	Error or Warning	Troubleshooting Approach/Explanation
3000	Fatal error in HFINTP, interpolation failed	The current time in VADOFT exceeds the supplied values of the interpolation time vector in attempting to interpolate head or flux values. This error should not occur when running VADOFT in linked mode. If running VADOFT alone, increase the number of time periods of the interpolation time and head/flux vectors.
3010	VARCAL - timestep nnn solution fails to converge after nnn reductions	The maximum number of time refinements was exceeded due to non-convergence. Relax the converge criterion, change the iterative scheme or revise VADOFT parameters.
3020	Attempt to run VADOFT w/PRZM on and ITRANS .ne.1	The user has attempted to run VADOFT with PRZM on and ITRANS not equal to one. Set ITRANS to 1 and make the appropriate changes to the VADOFT parameter file.
3030 3040	Incorrect value for IMODL in VADOFT input	An incorrect value has been entered for IMODL in the VADOFT input file. Check the values entered; IMODL = 0 for transport, IMODL = 1 for flow.
3050	Requested value of NOBSND [nnnn] greater than MXPRT [nnnn]	The value entered for the number of observation nodes in VADOFT (NOBSND) exceeds the maximum (MXPRT). Reduce the number of observation modes or increase MXPRT in the PARAMETER statement. If the latter, recompile the model.
3060	Transport simulation, NVREAD reset to 1	The value of NVREAD supplied by the user was reset to 1 since a transport simulation was requested; no action required.
3070	PRZM is on; IVSTED reset to 1	The value of IVSTED supplied by the user was reset to 1; no action required.

Table 8-1. RUSTIC ERROR MESSAGES, WARNINGS, AND TROUBLESHOOTING APPROACHES (continued)

	Error or Warning	Troubleshooting Approach/Explanation
3080	PRZM is on; flow boundary conditions will be overwritten	If PRZM is on and linked to VADOFT, a prescribed flux b.c. will be used at the VADOFT top node. Daily values of water and solute flux are generated by PRZM. Related boundary conditions in the VADOFT impact file are overwritten. IBTND1 is set to 0; no action required.
3090	PRZM is on; transient data at top node ignored	If PRZM is on, any transient flow data relevant to VADOFT's upper boundary is overwritten. ITCND1 is set to 0; no action required.
3100	SAFTMOD is on; flow b.c. at bottom node overwritten	If SAFTMOD is on, a prescribed head boundary condition is used for VADOFT's bottom boundary. The head is determined by SAFTMOD input. IBTNDN is set to 1; no action required.
3110	SAFTMOD is on; transient data at bottom ignored	If SAFTMOD is ON, any transient flow data input by the user relevant to VADOFT's lower boundary is overwritten. ITCNDN is set to 0. No action required.
3120	PRZM is on; transport boundary conditions will be overwritten	PRZM output will overwrite VADOFT upper boundary condition for solute transport. PRZM generates daily volume of solute flux. IBTNDI is set to 0. No action required.
3130	PRZM is on; transient data at top node ignored	If PRZM is on, any transient solute flux data the user has input for the upper boundary in VADOFT is ignored. ITCNDN is set to 0. No action required.
3140 3150	SAFTMOD is on; transport b.c. at bottom node overwritten	If SAFTMOD is on, then the user defined b.c. for the lower VADOFT boundary is overwritten. A zero concentration boundary is used. IBTNDN is set to 1. No action required.

Table 8-1. RUSTIC ERROR MESSAGES, WARNINGS, AND TROUBLESHOOTING APPROACHES (continued)

	Error or Warning	Troubleshooting Approach/Explanation
3160	SAFTMOD is on, transient data at bottom ignored	If SAFTMOD is on, any transient data relevant to VADOFT's lower boundary is ignored. ITCNDN is set to 0. No action required.
3170	Invalid index [nnn] in reading PINT	An invalid index (less than 1 or greater than the parameter NP) was supplied for an initial condition value. Supply proper value.
3180	NTOMT<NLDLT in linked mode, NTOMT reset to <value>	The supplied value of NTOMT in the VADOFT input file was less than the value of NLDLT supplied for the execution supervisor. NTOMT has been reset to NLDLT. No action necessary but check the VADOFT echo of 'LIST OF BACKUP FILE OUTPUT MARKER TIME VALUES' to ensure that the integer day numbers from 1 to NLDLT are greater than or equal to the values in this list. If not, a read error of Darcy velocities may occur.
3190	ITMGEN<>1 in linked mode, results may be unpredictable	The user is supplying output marker time values which, potentially, could result in a read error of Darcy velocities during the VADOFT transport simulation.
3200	NTS reset to EXESUP supplied value (NLDLT) [<value>]	No action necessary. The value of NTS in the VADOFT input file will be overwritten by the value of NLDLT supplied to the execution supervisor input.
3210	End of file reading VADOFT Darcy velocities	Check to see if warning 3180 or 3190 occurred prior to this fatal error. Make necessary changes to VADOFT input file.
4000	Daughter products not currently implemented for aquitards	The model is currently only configured to run daughter products simulation in a single aquifer system. They cannot be simulated in aquitards or the lower of a two aquifer system.
4010	Invalid IRZON value [<value>] reading group <record no.>	A value for IRZON has been entered which is less than or equal to zero or which is greater than the maximum number of nodes. Check input sequence.

Table 8-1. RUSTIC ERROR MESSAGES, WARNINGS, AND TROUBLESHOOTING APPROACHES (continued)

	Error or Warning	Troubleshooting Approach/Explanation
4020	Flow simulation with IMODL.NE.1	User is attempting to run a flow simulation (SAFTMOD is on) with IMODL not equal to one. Reset IMODL to 1 in the SAFTMOD input file.
4030	Transport simulation with IMODL.NE.1	The value of IMODL is not set to zero in the SAFTMOD transport input file (SAFTMOD is on). Reset IMODL to 0 in the SAFTMOD input file.
4040	Value specified for NP [nnn] greater than max allowed [nnn]	The number of nodes in SAFTMOD exceeds the maximum value (MXNP). Decrease the number of nodes (and elements) in the SAFTMOD input file or increase MXNP in the PARAMETER statement. If the latter, recompile the code.
4050	No. of aquifer elements [nnn] not as specified [nnn]	The number of elements calculated by the mesh generator is not equal to the number in the input file. Recheck NE in the input file.
4060	IEXEC is zero in SAFTMOD	The program has terminated at the user's request because IEXEC = 0. Set IEXEC = 1 for the program to proceed after mesh generation is done.
4070	Daughter products not implemented for multiple aquifers	Daughter products (ICHAIN = 1) can only be simulated in a single aquifer system. Set ICHAIN to zero in the SAFTMOD parameter file.
4080	Default values of Darcy velocities will be overwritten	For a transport simulation in the linked system, default Darcy velocities will be overwritten. NUREAD is reset to 1. No action required.
4090	SAFTMOD input error reading group <record number>	The format in the input file does not match the format for the indicated group. Most likely, the preceeding group has additional or missing records. Check the SAFTMOD input file.

Table 8-1. RUSTIC ERROR MESSAGES, WARNINGS, AND TROUBLESHOOTING APPROACHES (continued)

	Error or Warning	Troubleshooting Approach/Explanation
4100	Invalid IPSZO value [<value>] reading group <record no.>	A value for IPSZO has been entered which is less than or equal to zero or which is greater than the maximum number of zones. Check <record no.> in input sequence.
5000	Format error in reading Monte Carlo input file	Check Monte Carlo input file. Illegal characters are in inappropriate data file columns.
5010	Premature end of Monte Carlo input file	Check Monte Carlo input file. Insufficient data lines have been provided given the users problem definition.
5020	Uniform random number could not be generated for exponential distribution	Random exponential distribution variates could not be generated. Probable cause is inappropriate distribution parameters being supplied in the Monte Carlo input file.
5030	Cannot have a negative mean for a log normal distribution. Mean equals <value>	A negative mean was calculated for a log normal distribution. Check distribution parameters supplied in the Monte Carlo input file.
5040	Subroutine DECOMP terminated, matrix BBT is not positive definite	Monte Carlo solution matrix could not be decomposed. Check distribution parameters supplied in Monte Carlo input file.
5050	The number of [MONTE CARLO RUNS] is greater than maximum of <value>	Too large a value was chosen for the number of Monte Carlo runs. Reduce number in input file or change NRMAX in parameter file and recompile.
5060	The number of [MONTE CARLO VARIABLES] is greater than maximum of <value>	Reduce number in input file or change MCMAX and recompile.
5070	The number of [EMPIRICAL DIST. DATA POINTS] is greater than maximum of <value>	Reduce number in input file or change NEMP and recompile.

Table 8-1. RUSTIC ERROR MESSAGES, WARNINGS, AND TROUBLESHOOTING APPROACHES (concluded)

	Error or Warning	Troubleshooting Approach/Explanation
5080	The number of [MONTE CARLO OUTPUT VARIABLES] is greater than maximum of <value>	Reduce number in input file or change NMAX and recompile.
5090	The number of [DAYS IN OUTPUT AVG. PERIOD] is greater than maximum of <value>	Reduce number in input file or change NPMAX and recompile.
5100	The number of [REQUESTED OUTPUT CDFS] is greater than maximum of <value>	Reduce number in input file or change NCMAX and recompile.
5110	First element for horizon [<value>] not found	The PRZM horizon value provided for a variable defined in the Monte Carlo input file is probably invalid (does not match the PRZM horizon/element number description provided in the PRZM input file).

Table 8-2. EXESUP PROGRAM VARIABLES

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
AVHEAD	m	Array	Average head in a recharge zone of the top SAFTMOD aquifer.	EXESUP	LNKSTO	M
AVSFLX	ppb m day^{-1}	Array	Average solute flux to the saturated zone over the SAFTMOD timestep.	EXESUP	LNKSTO	M
AVWFLX	cm day^{-1}	Array	Average water flux to the saturated zone over the SAFTMOD timestep.	EXESUP	LNKSTO	M
AVZWT	m	Array	Average water table elevation in a recharge zone of the top SAFTMOD aquifer.	EXESUP	LNKSTO	M
BASEND	--	Scalar	Number of bottom PRZM node within a given PRZM zone.	EXESUP	--	M
BOTFLX	cm day^{-1}	Array	Water flux from VADOFT base node for each timestep.	EXESUP	VADSTO	M
DAFLUX	q cm^{-2} day^{-1}	Array	Dispersive-advective flux at each PRZM node in each zone for each chemical (positive).	EXESUP	PRZSTO	M
DAVFLX	ppm cm day^{-1}	Array	Nodal values of dispersive advective flux from VADOFT.	EXESUP	VADSTO	M
DISUNS	ppm (q cm^{-3})	Array	Temporary storage of VADOFT (or PRZM) nodal concentrations for mass correction computations.	EXESUP	--	M
EDAT	--	Array	Ending day, month, year of PRZM simulation.	EXESUP	--	M
FLOSIM	--	Logical	Flow simulation indicator.	EXESUP	--	M
ICHEM	--	Scalar	Counter for number of chemicals.	EXESUP	--	M
IDAY0	--	Scalar	Starting day of PRZM simulation.	EXESUP	--	M

Table 8-2. EXESUP PROGRAM VARIABLES (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ILDLT	--	Scalar	Counter for PRZM or VADOFT timesteps within a SAFTMOD timestep.	EXESUP	--	M
IMON0	--	Scalar	Starting month of PRZM simulation.	EXESUP	--	M
IPRZM	--	Scalar	Counter for number of PRZM zones.	EXESUP	--	M
IPZONE	--	Scalar	Counter for VADOFT zones.	EXESUP	--	M
ISZONE	--	Scalar	Counter for SAFTMOD recharge zones.	EXESUP	--	M
ITSAFT	--	Scalar	Counter for SAFTMOD timesteps.	EXESUP	--	M
IYR0	--	Scalar	Starting year of PRZM simulation.	EXESUP	--	M
MFLX	cm day^{-1}	Array	Chemical efflux from bottom (equivalenced with WFLX).	EXESUP	LNKSTO	M
LLSTS	days	Scalar	Number of days in final SAFTMOD timestep.	EXESUP INITEM	--	I O
NCHEM	--	Scalar	Number of chemicals.	EXESUP INPREA INITEM	--	I I O
NDAYS	days	Scalar	Number of days in a SAFTMOD timestep minus one.	EXESUP	--	M
NLDLT	--	Scalar	Number of PRZM or VADOFT timesteps within a SAFTMOD timestep.	EXESUP INPREA INITEM	--	I I O
NP	--	Scalar	Total number of SAFTMOD nodes.	EXESUP	CONTR2	I
NPNARY	--	Array	Number of VADOFT nodes in all VADOFT zones.	EXESUP	--	M

Table 8-2. EXESUP PROGRAM VARIABLES (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NPRZM	--	Scalar	Number of PRZM zones.	EXESUP INPREA INITEM	--	I I O
NPV	--	Scalar	Number of VADOFT nodes in a given zone.	EXESUP	--	I
NPZONE	--	Scalar	Number of VADOFT zones.	EXESUP INPREA INITEM	--	I I O
NPZ	--	Scalar	Temporary storage for the amount number of PRZM or VADOFT nodes.	EXESUP	--	M
NSZONE	--	Scalar	Number of SAFTMOD recharge or pesticide flux zones.	EXESUP INPREA INITEM	--	I I O
NTSAFT	--	Scalar	Number of SAFTMOD timesteps.	EXESUP INITEM	--	I O
PINT	L M/L**3	Array	VADOFT corrected values of head or concentration.	EXESUP	VADSTO	M
PRZMON	--	Logical	PRZM on indicator.	EXESUP INPREA INITEM	--	I I O
PRZMPF	q cm^{-2} day^{-1}	Array	Daily chemical flux from the base of PRZM.	EXESUP	PRZSTO	M
PRZMWF	cm day^{-1}	Array	Daily water flux from the base of PRZM.	EXESUP	PRZSTO	M
P2SWHT	--	Array	Weight for transfer of water or chemical flux from PRZM to SAFTMOD.	EXESUP	ZONWHT	M
P2VWHT	--	Array	Weighting factors for transfer of water or chemical flux from PRZM to VADOFT.	EXESUP	ZONWHT	M
REDAT	--	Array	Ending day, month, year of PRZM simulation within a given SAFTMOD timestep.	EXESUP	--	M

Table 8-2. EXESUP PROGRAM VARIABLES (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
RSDAT	--	Array	Starting day, month, year of PRZM simulation within a given SAFTMOD timestep.	EXESUP	--	M
RSTFG	--	Scalar	PRZM restart flag, 1 if first time through, 2 thereafter.	EXESUP	--	M
SAFTON	--	Logical	SAFTMOD on indicator.	EXESUP INPREA INITEM	--	I I O
SAVCNC	ppm	Array	Concentrations at each VADOFT node from previous timestep.	EXESUP	VADSTO	M
SAVHED	cm	Array	Previous timestep VADOFT heads by node.	EXESUP	VADSTO	M
SDAT	--	Array	Starting day, month, year of PRZM simulation.	EXESUP	--	M
SFLDT	ppm cm day^{-1} (gcm^{-2} day^{-1})	Array	Interpolated values of solute flux at the water table by zone and timestep for VADOFT (PRZM).	EXESUP	LNKSTO	M
SVSCNC	ppb	Array	Nodal concentrations from previous SAFTMOD timestep.	EXESUP	SFTSTO	M
SVSHED	m	Array	Initial head values for SAFTMOD.	EXESUP	SFTSTO	M
TIME1	days	Scalar	Beginning time of current SAFTMOD timestep.	EXESUP	--	M
TIME2	days	Scalar	Ending time of current SAFTMOD timestep.	EXESUP	--	M
TOPFLX	cm day^{-1} (μg cm^{-2} day^{-1})	Array	Weighted water (or pesticide) flux leaving the base of PRZM.	EXESUP	VADSTO	M
TOWFLX	cm day^{-1}	Array	Water flux from PRZM to top of VADOFT for each timestep.	EXESUP	VADSTO	M

Table 8-2. EXESUP PROGRAM VARIABLES (concluded)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
TRNSIM	--	Logical	Indicator for flow and transport simulation.	EXESUP INPREA INITEM	--	I I O
TRTERM	$\mu g\ cm^{-2}\ day^{-1}$	Array	Chemical decay within VADOFT nodes	EXESUP	VCHMDK	M
TRTERM	$ppb\ m\ day^{-1}$	Array	Chemical decay within SAFTMOD nodes	EXESUP	SCHMDK	M
VADFON	--	Logical	VADOFT on indicator.	EXESUP INPREA INITEM	--	I I O
VD2TC	--	Array	VADOFT correction factors for converting from dissolved to total solute concentration.	EXESUP	VADSTO	M
V2SWHT	--	Array	Weight for transfer of water or chemical flux from VADOFT to SAFTMOD.	EXESUP	--	M
WFLX	$cm\ day^{-1}$	Array	Water efflux from bottom (equivalenced with MFLX).	EXESUP	LNKSTO	M
WHGT	--	Scalar	Temporary variable for storing flux weighting factors.	EXESUP	--	M
WTZLT	m	Array	Daily interpolated value of water table elevation within the SAFTMOD timestep.	EXESUP	LNKSTO	M
ZPESTR	$g\ cm^{-2}\ day^{-1}$	Array	PRZM chemical flux by zone, compartment, time period, and chemical.	EXESUP	PRZSTO	M

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
A	day^{-1}	Array	Lower Diagonal Element of Solution Matrix (I-1)	SLPST0	PEST	O
				SLPST1		O
				TRDIAG		I
AAA	cm^{-1}	Scalar	A Variable Used to Calculate the Average Temperature Gradient in the Top Compartment	SLTEMP		M
ABSOIL	fraction	Scalar	Daily Value of Soil Surface Albedo	SLTEMP		M
AD	day^{-1}	Array	Soil Horizon Drainage Parameter	PRZMRD	HYDR	O
				ECHO		I
				INITL		I
				HYDR2		I
ADFLUX	$g\ cm^{-2}\ day^{-1}$	Array	Advective Flux of Pesticide	SLPST0	PEST	O
				SLPST1		O
				OUPPST		I
				OUTTSR		I
				MASBAL		I
ADS	$mg\ kg^{-1}$	Array	Adsorbed Portion of Pesticide in Each Compartment	OUTCNC		
AFIELD	ha	Scalar	Area of Field	PRZMRD	HYDR	O
				EROSN		
AINF	cm	Array	Percolation Into Each Soil Compartment	HYDR0L	HYDR	O
				HYDR1		I
				HYDR2		I
AIRDEN	$gm\ cm^{-3}$	Scalar	Density of Air at Ambient Temperature	SLTEMP		M
AIRLMD	$cal\ cm^{-1}\ day^{-1}\ °C^{-1}$	Scalar	Thermal Conductivity of Air	SLTEMP		
AKAY	--	Array	K-Factor in the Soil Thermal Conductivity Equation	SLTEMP		M

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ALAMDA	cal cm^{-1} day^{-1} °C^{-1}	Array	Thermal Conductivity of Soil Constituent	SLTEMP		
ALBEDO	fraction	Array	Soil Surface Albedo at Start of Each Month	PRZMRD SLTEMP	MET	O I
AMXDR	cm	Scalar	Maximum Rooting Depth of Each Crop	PRZMRD INITL PLGROW	CROP	O I I
ANETD	cm	Scalar	Minimum Depth from Which ET is Extracted Year Around	PRZMRD INITL	CROP	O I
ANUM	cm	Scalar	Total Available Water in Profile	EVPOTR		
APD	--	Scalar	Day of Month of Pesticide Application	PRZMRD		
APDEP	cm	Scalar	Depth of irrigation water applied to soil	IRRIG	--	O
APM	--	Scalar	Month of Pesticide Application	PRZMRD		
ATEMP	°C	Array	Air Temperature	Main		O
AVSTOR	cm^{3} cm^{-3}	Scalar	Available Water Storage	HYDR2		
AW	--	Scalar	Fraction of Soil Voids Occupied by Water	EVPOTR		
B	day^{-1}	Array	Diagonal Element of Solution Matrix (I)	SLPST0 SLPST1 TRDIAG	PEST	O
BBB	°K cm^{-1}	Scalar	A Variable Used to Calculate the Average Temperature Gradient in the Top Compartment	SLTEMP		M
BBT	°C	Array	Bottom Boundary Temperature at Start of Each Month	PRZMRD SLTEMP	MET	O I

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
BD	g cm^{-3}	Array	Mineral Soil Bulk Density	SLTEMP	HYDR	I
BDFLAG	--	Scalar	Bulk Density Flag (0 = Whole Soil BD Entered, 1 = Mineral BD and OC Entered)	PRZMRD ECHO INITL		O I I
BT	m	Scalar	Bottom width of furrows	FURROW	IRGT	I
C	day^{-1}	Array	Upper Diagonal Element of Solution Matrix (I+1)	SLPST0 SLPST1 TRDIAG	PEST	O O I
CB	kg ha^{-1}	Scalar	Cumulative Pesticide Balance Error	OUTPST		
CC	g	Array	Total mass associated with a moving point	MOC INITL	PEST	M
CELLBG	--	Scalar	First location in a compartment	INITL		M
CEVAP	cm	Scalar	Current Daily Canopy Evaporation Depth	EVPOTR MASBAL OUTHYD OUTTSR	HYDR	O I I I
CFLAG	--	Scalar	Conversion Flag for Initial Pesticide Input	PRZMRD INITL	MISC	O I
CHANGE	g	Array	Change in total pesticide mass per compartment	MOC		M
CINT	cm	Scalar	Current Crop Interception Storage	INITL HYDROL EVPOTR MASBAL OUTHYD OUTTSR	HYDR	O I I I I I
CINTB	cm	Scalar	Crop Interception From Previous Time Step	PRZM MASBAL OUTHYD	HYDR	O I I

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
CINTCP	cm	Array	Maximum Interception Storage of Each Crop	PRZMRD ECHO PLGROW	CROP	O I I
CLAY	percent	Array	Percent Clay in Each Soil Horizon	SLTEMP	HYDR	I
CONC	--	Alpha-numeric	Flag for Output of Soil Pesticide Concentration Profile	PRZM		
CONDUC	cm day^{-1}	Scalar	Canopy Conductance Including Boundary Layer's Conductance	PRZM SLPST0 SLPST1	PEST	O I I
CONST	--	Scalar	Constant Values Used to Multiply Each Time Series Output	PRZMRD ECHO OUTTSR		O I I
CORED	cm	Scalar	Total Depth of Soil Profile	PRZMRD ECHO INITL	HYDR	O I I
COVER	fraction	Scalar	Current Areal Cover of Crop Canopy	SLTEMP	CROP	I
COUNT	--	Array	Number of moving points in a compartment	MOC		M
COVMAX	fraction	Array	Maximum Areal Coverage of Each Crop at Full Canopy Development	PRZMRD ECHO INITL PLGROW	CROP	O I I I
CN	--	Array	Runoff Curve Numbers for Antecedent Soil Moisture Condition II	PRZMRD ECHO HYDROL	HYDR	O I I
CNCPND	g cm^{-3}	Scalar	Concentration of pesticide in inflowing water	MOC INITL	PEST	I
CNDBDY	cm day^{-1}	Scalar	Boundary Layer's Conductance	PRZM		O

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
CNDM	--	Array	Accumulated Number of Days in Each Month (With and w/o Leap Year)	PRZM		
CNDMO	--	Array	Accumulated Number of Days in Each Month	SLTEMP	MISC	I
CPBAL	g cm^{-2}	Scalar	Cumulative Pesticide Balance Error	MASBAL OUTPST	PEST	M I
CRC	day m^{-1}	Array	Canopy Resistance	CANOPY		O
CRCNC	day m^{-1}	Array	Canopy Resistance	PRZM OUTPST	PEST	I O
CTOT	g	Scalar	Concentration of consolidated points	MOC	--	M
CURVN	--	Scalar	Current Value of Runoff Curve Number	HYDROL		
CWBAL	cm	Scalar	Cumulative Water Balance Error	MASBAL OUTHYD	HYDR	M I
D	m	Scalar	Zero Displacement Height	CANOPY SLTEMP		O M
DAIR	cm^2 day^{-1}	Scalar	Molecular Diffusivity in the Air	ECHO PRZM PRZMRD SLPST0 SLPST1	PEST	I I O I I
DAY	--	Alpha-numeric	Flag for Daily Output of Water or Pesticide Summary	PRZM		
DELT	day	Scalar	Time Step	INITL HYDR2 PLPEST SLPST0 SLPST1 MASBAL	MISC	O I I I I I

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
DELTA	°K	Scalar	Convergence Criteria in the Newton-Raphson Solution Technique	SLTEMP		M
DELX	cm	Array	Compartment Thickness	SLTEMP	HYDR	I
DELXSQ	cm^{-2}	Scalar	Compartment Thickness Squared	INITL SLPST0 SLPST1	HKYDR	O
DEN	-	Array	Point density. The number of points in the horizon divided by the depth of the horizon.	INITL	HYDR	M
DENOM	cm	Scalar	Total Voids in the Soil Profile	EVPOTR		
DENOM	$cm\ hr^{-1}$	Scalar	Available Water for Runoff During a Storm	EROSN		
DEPI	cm	Array	Depth of Pesticide Incorporation	PRZMRD ECHO PESTAP	PEST	O I
DFFLUX	$g\ cm^{-2}\ day^{-1}$	Array	Diffusive/Dispersive Flux of Pesticide Leaving Each Soil Compartment	SLPST0 SLPST1 OUTPST OUTTSR	PEST	O O I I
DGAIR	$cm^2\ day^{-1}$	Array	Molecular Diffusivity in the Soil Air Pore	SLPST0 SLPST1		I I
DGRATE	day^{-1}	Array	First Order Decay Rate for Vapor-Phase Pesticide	ECHO INITL PRZMRD SLPST0 SLPST1	PEST	I I O I I
DIFFCH	$m^2\ day^{-1}$	Scalar	Eddy Diffusivity at Canopy Height	CANOPY		O
DIFFCO	$cm^2\ day^{-1}$	Array	Diffusivity of Soil Compartment	SLTEMP		M

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
DIFK	m^2 day^{-1}	Scalar	Eddy Diffusivity	CANOPY		O
DIN	cm	Scalar	Current Plant Canopy Interception Potential	PLGROW	HYDR	O
				HYDROL		I
				OUTHYD		I
DISP	cm^2 day^{-1}	Array	Dispersion/Diffusion Coefficient	PRZMRD	PEST	O
				ECHO		I
				INITL		I
				SLPST0		I
				SLPST1		I
DISS	mg l^{-1}	Array	Dissolved Portion of Pesticide in Each Compartment	OUTCNC		
DKFLUX	g cm^{-2}	Array	Decay Flux of Pesticide From Each Compartment	SLPST0	PEST	O
				SLPST1		O
				MASBAL		I
				OUTPST		I
				OUTTSR		I
DKRATE	day^{-1}	Array	Pesticide Decay Rate in Each Soil Horizon	PRZMRD	PEST	O
				ECHO		I
				INITL		I
				SLPST0		I
				SLPST1		I
DKRT12	day^{-1}	Array	Transformation Rate from Parent Pesticide to First Daughter Product	ECHO	PEST	I
				PRZMRD		O
				INITL		O
				PSTLNK		I
DKRT13	day^{-1}	Array	Transformation Rate from Parent Pesticide to Second Daughter Product	ECHO	PEST	I
				PRZMRD		O
				INITL		O
				PSTLNK		I
DKRT23	day^{-1}	Array	Transformation Rate from First Daughter Product to Second Daughter Product	ECHO	PEST	I
				PRZMRD		O
				INITL		O
				PSTLNK		I

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
DOM	--	Scalar	Number of Current Day of Month of Simulation	SLTEMP	MISC	I
DPN	cm	Array	Layer Depth in Each Horizon	ECHO PRZMRD	HYDR	I O
DT	hr	Array	Average Hours of Daylight for a Day Falling in Each Month	PRZMRD ECHO EVPOTR	MET	O I I
DVF	kg ha^{-1} day^{-1}	Scalar	Daily Foliage Pesticide Volatilization Flux	OUTPST		O
DW	Fraction	Scalar	Available porosity in soil column	IRRIG FURROW	IRGT	O
DX	m	Scalar	Spatial stop used in furrow finite difference model	FURROW IRRIG	IRGT	M I
EF	kg ha^{-1}	Scalar	Daily Erosion Flux	OUTPST		
ELTERM	day^{-1}	Scalar	Erosion Loss Term for Pesticide Balance	EROSN SLPST0 SLPST1	PEST	O I I
EMD	--	Scalar	Day of Month of Crop Emergence	PRZMRD ECHO		
EMM	--	Scalar	Month of Crop Emergence	PRZMRD ECHO		
EMMISS	fraction	Scalar	Infrared Emissivity of Soil Surface	PRZMRD SLTEMP	MET	O I
EN	--	Scalar	Manning's roughness coefficient for furrows	FURROW	IRGT	I
ENP	Kcal $mole^{-1}$	Scalar	Enthalpy of Vaporization	KHCORR		I
ENPY	Kcal $mole^{-1}$	Array	Enthalpy of Vaporization	ECHO PRZM PRZMRD	PEST	I I O

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ENRICH	--	Scalar	Enrichment Ratio for Organic Matter	EROSN		
ERFLAG	--	Scalar	Erosion Flag (0= Not Calculated, 1= Calculated)	PRZMRD PRZM	HYDR	O I
ERFLUX	g cm^{-2}	Scalar	Erosion Flux of Pesticide From Soil Surface	SLPST0 SLPST1 MASBAL OUTPST	PEST	O O I I
EVAP	cm day^{-1}	Scalar	Daily Evaporation from the Top 5 cm of Soil After Adjusting for Crop evapotranspiration	SLTEMP		M
EXTRA	$\mathrm{cm}^3\ \mathrm{cm}^{-3}$	Scalar	Extra Water Occurring in a Compartment Over the Allowed Saturation Amount	OUTTSR HYDR2		I
F	g cm^{-2} day^{-1}	Array	Vector of Source Terms for Each Compartment (Tri-diagonal Matrix)	SLPST0 SLPST1 TRDIAG	PEST	O O I
FO/	kg ha^{-1}	Scalar	Current Foliar Pesticide Storage	OUTPST		
FAIH	--	Scalar	Stability Function for Sensible Heat	CANOPY		O
FAIM	--	Scalar	Stability Function for Momentum	CANOPY		O
FAM	--	Scalar	Pesticide Application Flag (1= Soil, 2= Linear Foliar, 3= Exponential Foliar)	PRZMRD ECHO PESTAP	PEST	O I I
FC	cm	Array	Field Capacity Water Depth in Soil Compartment	INITL EVPOTR	HYDR	O

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
FCV	--	Array	Regression Coefficients for Prediction of Field Capacity Soil Water Content	THCALLC		
FDAY	--	Scalar	Loop Limit, First Day	PRZM		
FEXTRC	cm^{-1}	Scalar	Foliar Extraction Coefficient for Foliar Wash-off Model	PRZMRD ECHO PLPEST	PEST	O I I
FILTRA	$m^2\ kg^{-1}$	Scalar	Filtration Parameter for Exponential Foliar Application Model	PRZMRD ECHO PESTAP	PEST	O I I
FIRST	-	Scalar	Index of first point under interface with Ratio greater than 2	MOC	HYDR	M
FL	$kg\ ha^{-1}$	Scalar	Foliar Pesticide Decay Loss	OUTPST		
FLEACH	Fraction	Scalar	Leaching factor, as fraction of soil moisture deficit	IRRIG	IRGT	I
FOLPO/	$g\ cm^{-2}$	Scalar	Foliar Pesticide Storage From Previous Time Step	PLPEST MASBAL OUTPST PRZM	PEST	O I I I
FP	$kg\ ha^{-1}$	Scalar	Current Daily Foliar Pesticide Storage	OUTPST		
FPDLOS	$g\ cm^{-2}$	Scalar	Current Daily Foliar Pesticide Decay Loss	PLPEST MASBAL OUTPST OUTTSR	PEST	O I I I
FPVLOS	$g\ cm^{-2}\ day^{-1}$	Array	Daily Foliage Pesticide Volatilization Flux	MASBAL OUTPST PLPEST	PEST	I I O

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
FPWLOS	g cm^{-2}	Scalar	Current Daily Pesticide Washoff Loss	PLPEST		
FRAC	--	Scalar	Fraction of the Distance a Curve Number is Between Increments of Ten	PRZMRD		
FRAC	--	Scalar	Fraction of the Current Crop Growing Season Completed	PLGROW		
FRAC	--	Array	Number of Compartments Available to Extraction of ET	EVPOTR		
FRACOM	--	Scalar	Fraction of Layer Attributed to the Current Horizon	INITL		
FS	m	Array	Infiltration depth at each station in furrow	FURROW IRRIG	IRGT	O I
FX1	$°K^4$	Scalar	Fourth Order Energy Balance Equation in Terms of Soil Surface Temperature	SLTEMP		M
FX2	$°K^3$	Scalar	Derivative of Energy Balance Equation in Terms of Soil Surface Temperature	SLTEMP		M
GAMMA	--	Array	Pesticide Uptake Efficiency by Plant	PLGROW SLPST0 SLPST1	PEST	O I I
GEE	Fraction	Array	Depolarization Factors of Soil Constituent in Three Dimensions	SLTEMP		M
GFLD	Fraction	Scalar	Depolarization Factor of Entrapped Air at Field Capacity Water Content	SLTEMP		M

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
GRADT	°C m^{-1}	Scalar	Temperature Gradient	CANOPY		O
GRADW	day^{1}	Scalar	Wind Speed Gradient	CANOPY		O
HAD	--	Scalar	Day of Month of Crop Harvest	PRZMRD ECHO		
HAM	--	Scalar	Month of Crop Harvest	PRZMRD ECHO		
HEIGHT	cm	Scalar	Canopy Height	PRZM OUTPST PLGROW SLTEMP	CROP	I I O I
HENRY	$cm^3\ cm^{-3}$	Scalar	Henry's Constant	KHCORR		I
HENRYK	$cm^3\ cm^{-3}$	Array	Henry's Constant	ECHO PRZM PRZMRD	PEST	I I O
HF	m	Scalar	Green-Ampt Suction head parameter	FURROW INFIL	IRGT	I I
HGT	m	Scalar	Thickness of Each Layer in the Canopy	CANOPY		O
HORIZN	--	Array	Soil Horizon Number	PRZMRD ECHO INITL OUTHYD OUTPST OUTCNC	MISC	O I I I I I
HSWZT	--	Scalar	Hydraulics Flag (0= Free Draining Soils, 1= Restricted Drainage)	PRZMRD ECHO INITL PRZM		O I I I
HTEMP	°C	Scalar	Average Air Temperature	CANOPY		O
HTITLE	--	Alpha-numeric	Comment Line to Enter Information about Hydrology Parameters	PRZMRD ECHO		

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
HTMAX	cm	Array	Maximum Canopy Height	ECHO PLGROW PRZMRD	CROP	I M O
I	--	Scalar	Loop Counter	SLTEMP KHCORR CANOPY		
IAPDY	--	Array	Julian Day of Pesticide Application	PRZMRD ECHO PRZM	MISC	O I I
IAPYR	--	Array	Year of Pesticide Application	PRZMRD ECHO PRZM	MISC	O I I
IARG	--	Array	Argument of Variable Identified by 'PLNAME'	PRZMRD ECHO OUTTSR	MISC	O I I
IARG1	--	Scalar	Argument of Variable Identified by 'PLNAME'	OUTTSR		
IB	--	Scalar	Backward Loop Index	INITL HYDR2		
IBM1	--	Scalar	Counter	INITL		
ICNAH	--	Array	Soil Surface Condition After Harvest	PRZMRD ECHO PLGROW	HYDR	O I I
ICNCN	--	Array	Crop Number	PRZMRD ECHO INITL PLGROW	CROP	O I I I
ICROSS	--	Scalar	Number of horizon interfaces where points need to be consolidated, i.e., Ratio greater than 2.	INITL MOC	HYDR	M
IDEL	--	Scalar	Number of points which are consolidated	MOC	-	M

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
IDFLAG	--	Scalar	Flag to Identify if Soil Thermal Conductivity and Heat Capacity are Input or Simulated in the Model	ECHO PRZMRD SLTEMP OUTCNC	MET	I O I I
IEDAY	--	Scalar	Ending Day of Simulation	PRZMRD PRZM ECHO	MISC	O I I
IEDY	--	Scalar	Counter	INITL		
IEMER	--	Array	Julian Day of Crop Emergence	PRZMRD ECHO INITL PLGROW	CROP	O I I I
IEMON	--	Scalar	Ending Month of Simulation	PRZMRD ECHO PRZM	MISC	O I I
IEND	--	Scalar	Index of point at which consolidation ends	MOC	-	M
IERROR	--	Scalar	Error Flag if Tri-Diagonal Matrix Cannot be Saved	SLPST0 SLPST1 TRDIAG		
IEYR	--	Scalar	Ending Year of Simulation	PRZMRD ECHO PRZM	MISC	O I I
IFIRST	--	Scalar	Flag to Print Output Heading and Initialize Output Array	OUTTSR		
IHAR	--	Array	Julian Day of Crop Harvest	PRZMRD ECHO INITL PLGROW	CROP	O I I I
II	--	Scalar	Loop Counter	OUTPST		
IJ	--	Scalar	Loop Counter	PRZM		

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ILP	--	Scalar	Initial Level of Pesticide Flag (0= No Pesticide, 1= Initial Pesticide)	PRZMRD ECHO	MISC	O I
INABS	cm	Scalar	Initial Abstraction of Water from Potential Surface Runoff	HYDROL EROSN	HYDR	O I
INCROP	--	Array	Crop Growing in Current Cropping Period	PRZMRD ECHO INITL PLGROW OUTHYD OUTPST	CROP	O I I I I
INICRP	--	Scalar	Initial Crop Number if Simulation Starting Date is Before First Crop Emergence Date	PRZMRD ECHO INITL	CROP	O I I
INTFC	--	Scalar	Whole Layer(s) Attributed to the Current Horizon	INITL		
IOUT	--	Scalar	Index of first point outside flow domain	MOC		M
IPEIND	--	Scalar	Pan Evaporation Indicator Flag (0= Data Read In, 1= Calculated)	PRZMRD ECHO	MET	O I
IPSCND	--	Scalar	Foliage Pesticide Condition after Harvest: 1. Surface Applied 2. Removed 3. Surface Residue	ECHO PLGROW PRZMRD	CROP	I M O
IRTYPE	--	Scalar	Irrigation type flag: 0=No irrigation 1=Flood irrigation 2=Furrow irrigation 3=Over-canopy sprinklers 4=Under-canopy sprinklers	IRRIG	IRGT	I

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ISCOND	--	Scalar	Surface Condition After Harvest Corresponding to 'INICRP'	PRZMRD	HYDR	O
				ECHO		I
				PLGROW		I
				HYDROL		I
				EROSN		I
ISDAY	--	Scalar	Starting Day of Simulation	PRZMRD	MISC	O
				ECHO		I
				INITL		I
				PRZM		I
ISDY	--	Scalar	Counter	INITL		
ISMON	--	Scalar	Starting Month of Simulation	PRZMRD	MISC	O
				ECHO		I
				INITL		I
				PRZM		I
ISTART	--	Scalar	Index of point at which consolidation starts	MOC	-	M
ISTYR	--	Scalar	Starting Year of Simulation	PRZMRD	MISC	O
				ECHO		I
				INITL		I
				PRZM		I
ITEM1	--	Alpha-numeric	Hydrology Output Summary Indicator	PRZMRD	MISC	O
				ECHO		I
				OUTHYD		I
ITEM2	--	Alpha-numeric	Pesticide Output Summary Indicator	PRZMRD	MISC	O
				ECHO		I
				OUTPST		I
ITEM3	--	Alpha-numeric	Soil Pesticide Concentration Profile Output Indicator	PRZMRD	MISC	O
				ECHO		I
				PRZM		I
ITEMP	°C	Scalar	Mean Daily Temperature Rounded to Next Lowest Whole Number	EVPOTR	MISC	O

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ITFLAG	--	Scalar	Soil Temperature Flag	ECHO PRZM OUTCNC PRZMRD	MET	I I I O
ITMP	--	Scalar	Number of Compartments Pesticide is Applied to When Incorporated	PESTAP		
IY	--		Annual Loop Counter	PRZM PLGROW OUTHYD OUTPST OUTTSR OUTCNC		I I I I I I
IYREM	--	Array	Year of Crop Emergence	PRZMRD ECHO INITL PLGROW	CROP	O I I I
IYRHAR	--	Array	Year of Crop Harvest	PRZMRD ECHO INITL PLGROW	CROP	O I I I
IYRMAT	--	Array	Year of Crop Maturation	PRZMRD ECHO INITL PLGROW	CROP	O I I I
J	--	Scalar	Loop Counter	PRZM PRZMRD ECHO INITL PLGROW OUTHYD OUTPST		
JJ	--	Scalar	Loop Counter	PRZMRD		
JP1	--	Scalar	Counter (J+1)	PRZMRD		
JP1T10	--	Scalar	Counter (JP1*10)	PRZMRD		

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
JT10	--	Scalar	Counter (J*10)	PRZMRD		
JULDAY	--	Scalar	Julian Day	PRZM PLGROW OUTHYD OUTPST	MISC	O I I I
K	--	Scalar	Loop Counter	SLTEMP		
KD	$cm^3\ g^{-1}$	Array	Adsorption/partition Coefficient for Soil Compartment	PRZMRD ECHO INITL KDCALC PESTAP SLPST0 SLPST1 MASBAL OUTPST OUTTSR OUTCNC	PEST	O I I O I I I I I I I
KDFLAG	--	Scalar	Partition Coefficient Flag (0= Kd Read In, 1= Kd Calculated)	PRZMRD ECHO PRZM		O I I
KH	$cm^3\ cm^{-3}$	Array	Henry's Constant at Current Time	PRZM SLPST0 SLPST1	PEST	O I I
KK	--	Scalar	Loop Counter	PRZMRD		I
KOC	$cm^3\ g^{-1}$ -oc	Scalar	Organic Carbon Partition Coefficient	KDCALC		
KS	m/s	Scalar	Saturated hydraulic conductivity of soil	FURROW INFIL	IRGT	I I
L	--	Scalar	Loop Counter	SLTEMP		
LAYERS	--	Scalar	Number of Layers in Canopy	CANOPY		O
LBTEMP	°C	Scalar	Daily Value of Bottom Boundary Temperature	SLTEMP		M

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
LDAY	--	Scalar	Loop Limit (Last Day)	PRZM		
LEAP	--	Scalar	Additional Day Flag for Leap Year	SLTEMP		I
LFREQ1	--	Scalar	Frequency of Soil Compartment Reporting in Water Output Summary	PRZMRD OUTHYD	MISC	O I
LFREQ2	--	Scalar	Frequency of Soil Compartment Reporting in Pesticide Output Summary	PRZMRD OUTPST	MISC	O I
LFREQ3	--	Scalar	Frequency of Soil Compartment Reporting in Concentration Profile Output Summary	PRZMRD OUTCNC	MISC	O I
LL	--	Scalar	Loop counter	MOC		
LOGD	--	Scalar	Logarithm of Zero Displacement Height	CANOPY		O
LOGKOC	--	Scalar	Natural Log of Koc	KDCALC		
LOGZO	--	Scalar	Logarithm of Roughness Length	CANOPY		O
M	--	Scalar	Loop counter	MOC		
MAD	--	Scalar	Day of Month of Crop Maturation	PRZMRD ECHO		
MAM	--	Scalar	Month of Crop Maturation	PRZMRD ECHO		
MASS	g	Array	Current pesticide mass in compartment	MOC		M
MASSO	g	Array	Total pesticide mass in each compartment at previous time step	MOC INITL	PEST	M

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
MAT	--	Array	Julian Day of Crop Maturation	PRZMRD ECHO INITL PLGROW	MISC	O I I I
MCFLAG	--	Scalar	Transport solution technique flag (0 = PRZM, 1= MOCPRZM)	ECHO PRZMRD PRZM	PEST	I
MD	--	Scalar	Number of Day Read from Meteorologic File	PRZM		
MDOUT	kg ha^{-1}	Array	Monthly Pesticide Decay from Each Compartment	OUTPST	ACCUM	M
MEOUTW	cm	Array	Monthly ET from Each Soil Compartment	OUTHYD	ACCUM	M
MINPP	kg ha^{-1}	Array	Monthly Advection/Dispersion Flux from Each Compartment	OUTPST	ACCUM	M
MINPP1	kg ha^{-1}	Scalar	Monthly Foliar Applied Pesticide	OUTPST	ACCUM	M
MINPP2	kg ha^{-1}	Scalar	Monthly Soil Applied Pesticide	OUTPST	ACCUM	M
MINPW	cm	Array	Monthly Infiltration into Each Soil Compartment	OUTHYD	ACCUM	M
MINPW1	cm	Scalar	Monthly Precipitation	OUTHYD	ACCUM	M
MINPW2	cm	Scalar	Monthly Snowfall	OUTHYD	ACCUM	M
MINTH	--	Alpha-numeric	Flag for Monthly Output Summary (for Either Water or Pesticide)	PRZM		
MM	--	Scalar	Number of Month Read from Meteorologic File	PRZM		
MNTHP1	--	Scalar	Current Month Plus 1 (Month + 1)	OUTHYD		

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
MODFC	--	Scalar	Fraction Multiplier	INITL		
MONTH	--	Scalar	Number of Current Month of Simulation	SLTEMP	MISC	I
MOUTP	kg ha^{-1}	Array	Monthly Pesticide Uptake from Each Compartment	OUTPST	ACCUM	M
MOUTP1	kg ha^{-1}	Scalar	Monthly Pesticide Washoff Flux	OUTPST	ACCUM	M
MOUTP2	kg ha^{-1}	Scalar	Monthly Pesticide Runoff Flux	OUTPST	ACCUM	M
MOUTP3	kg ha^{-1}	Scalar	Monthly Pesticide Erosion Flux	OUTPST	ACCUM	M
MOUTP4	kg ha^{-1}	Scalar	Monthly Foliar Pesticide Decay Loss	OUTPST	ACCUM	M
MOUTP5	kg ha^{-1}	Scalar	Monthly Pesticide Uptake Flux from Profile	OUTPST	ACCUM	M
MOUTP6	kg ha^{-1}	Scalar	Monthly Pesticide Decay Flux from Profile	OUTPST	ACCUM	M
MOUTW	cm	Array	Monthly Exfiltration from Each Compartment	OUTHYD	ACCUM	M
MOUTW1	cm	Scalar	Monthly Canopy Evaporation	OUTHYD	ACCUM	M
MOUTW2	cm	Scalar	Monthly Thrufall	OUTHYD	ACCUM	M
MOUTW3	cm	Scalar	Monthly Runoff	OUTHYD	ACCUM	M
MOUTW4	cm	Scalar	Monthly Snowmelt	OUTHYD	ACCUM	M
MOUTW5	cm	Scalar	Monthly Evapotranspiration	OUTHYD	ACCUM	M
MOUTW6	MTonne	Scalar	Total Monthly Sediment Loss	OUTHYD	ACCUM	

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
MSTART	--	Scalar	Flag for Positioning Meteorologic File	PRZM		
MSTR	cm	Array	Previous Month Storage of Water in Each Soil Compartment	OUTHYD	ACCUM	M
MSTR1	cm	Scalar	Monthly Canopy Interception	OUTHYD	ACCUM	M
MSTR2	cm	Scalar	Monthly Accumulation of Snow	OUTHYD	ACCUM	M
MSTRP	kg ha^{-1}	Array	Storage of Pesticide from Previous Month in Each Soil Compartment	OUTPST	ACCUM	M
MSTRP1	kg ha^{-1}	Scalar	Storage of Foliar Pesticide from Previous Month	OUTPST	ACCUM	M
MY	--	Scalar	Number of Year Read from Meteorologic File	PRZM		
N	--	Scalar	Loop Counter	CANOPY SLTEMP		
NAPPC	--	Scalar	Pesticide Application Counter	PRZM PESTAP	PEST	O I
NAPS		Scalar	Number of Pesticide Applications in the Simulation	PRZMRD ECHO INITL PRZM	PEST	O I I I
NBYR	--	Scalar	Beginning Year of Crop Growth for Current Crop (Loop Limit)	INITL PLGROW		
NCELL	--	Scalar	Compartment number in which a point is located	MOC INITL		M
NCOMO/	--	Scalar	Number of Compartments from Which ET is Extracted Year Round	INITL PLGROW	HYDR	O I

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NCOM1	--	Scalar	Current Number of Compartments, that ET is Extracted From	PLGROW EVPOTR OUTHYD	HYDR	O I I
NCOM2	--	Scalar	Number of Compartments in Soil Profile	SLTEMP	HYDR	I
NCOM2M	--	Scalar	Number of Compartments in Soil Profile Minus 1 (NCOM2 - 1)	INITL SLPST0 SLPST1	HYDR	O I I
NCOMRZ	--	Scalar	Number of Compartments in the Root Zone	INITL SLPST0 SLPST1 OUTHYD OUTPST	CROP	O I I I I
NCP	--	Scalar	Number of Current Cropping Period	INITL PLGROW	CROP	O I
NCPDS	--	Scalar	Number of Cropping Periods in the Simulation	PRZMRD ECHO INITL PLGROW	CROP	O I I I
NCROP	--	Scalar	Number of Current Crop	INITL PLGROW HYDROL EROSN	CROP	O I I I
NDC	--	Scalar	Number of Different Crops in Simulation	PRZMRD ECHO INITL PLGROW	CROP	O I I I
NDCNT	--	Scalar	Number of Days Since Crop Emergence for Current Crop	INITL PLGROW	MISC	O I
NDYRS	--	Scalar	Number of Years Between Emergence and Maturation of a Crop	INITL PLGROW		

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NET	g	Array	Net change in mass due to advection	MOC		M
NEW	--	Scalar	Number of new points entering the flow domain	MOC		M
NEWK	$cm^3\ cm^{-3}$	Array	Henry's Constant	KHCORR		O
NEXDAY	--	Scalar	Extra Day Added for Leap Year	PLGROW		
NEYR	--	Scalar	Ending Year of Crop Growth for Current Crop	INITL PLGROW		
NHORIZ	--	Scalar	Total Number of Soil Horizons	PRZMRD ECHO INITL KDCALC	MISC	O I I I
NLINES	--	Scalar	Numbers of Lines for Listing Initial Pesticides in Profile (Loop Limit)	ECHO		
NM1	--	Scalar	Number of Compartments in Profile Minus 1 (NCOM2 - 1)	TRDIAG		
NOPRT	--	Scalar	Print Flag	OUTHYD OUTPST		
NPI	--	Scalar	Current number of moving points in soil profile	MOC INITL	HYDR	M
NPLOTS	--	Scalar	Number of Time Series to be Output (Maximum of 7)	PRZMRD ECHO PRZM OUTTSR	MISC	O I I I
NRZCOM	--	Scalar	Current Number of Layers in Root Zone	PLGROW		
NSPACE	--	Scalar	Number of furrow stations for finite difference	FURROW IRRIG	IRGT	M I

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NSUM	--	Scalar	Cumulative Sum of Compartment Numbers	EVPOTR		
NSUMM	--	Scalar	Termination Loop Index for Summary Output	OUTHYD OUTPST		
NUM	--	Scalar	Number of Soil Compartment	KHCORR		I
NUM	--	Scalar	Intial number of moving points per compartment	MOC INITL	HYDR	I
NUMDYS	--	Scalar	Number of Days in a Month	SLTEMP		M
OC	percent	Array	Organic Carbon in Each Soil Horizon	SLTEMP	PEST	I
OKH	$cm^3\ cm^{-3}$	Array	Henry's Constant at Previous Time	INITL PRZM SLPST0 SLPST1	PEST	O I I I
ORGM	percent	Scalar	Organic Matter Content of a Soil Horizon	INITL		
OSNOW	cm	Scalar	Snow Accumulated at the End of the Previous Time Step	PRZM HYDROL MASBAL	HYDR	O I I
OUTPUT	--	Array	Output Array for Time Series	OUTTSR		
PA	$kg\ ha^{-1}$	Scalar	Daily Foliar Pesticide Application	OUTPST		
PB	$kg\ ha^{-1}$	Scalar	Pesticide Balance	OUTPST		
PBAL	$g\ cm^{-2}$	Scalar	Current Pesticide Balance Error	MASBAL OUTPST	PEST	O
PCDEPL	Fraction	Scalar	Fraction of available water capacity where irrigation is triggered	IRRIG	IRGT	I

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
PCMC	--	Scalar	Partition Coefficient Model Flag (1= Karickhoff, 2= Kenega, 3= Chiou)	PRZMRD KDCALC	MISC	O I
PCOUNT	--	Array	Number of points crossing an interface with Ratio greater than 2.	INITL MOC	HYDR	M
PESTR	g cm^{-3}	Array	Total Pesticide in Each Soil Compartment	PRZMRD ECHO INITL PRZM PESTAP MASBAL OUTPST	PEST	O I I I I I I
PET	cm	Scalar	Total Daily Potential Evapotranspiration	EVPOTR		
PETP	cm	Scalar	Running Total of Available Evapotranspiration	EVPOTR		
PEVP	cm	Scalar	Pan Evaporation	PRZM EVPOTR	MET	O I
PFAC	--	Scalar	Pan Factor for ET	PRZMRD ECHO EVPOTR	MET	O I I
PI	--	Scalar	3.1415926	CANOPY		
PLDKRT	day^{-1}	Array	Foliar Pesticide Decay Rate	PRZMRD ECHO PLPEST	PEST	O I I
PLNAME	--	Alpha-numeric	Time Series Output Identifier (Options Listed in User's Guide)	PRZMRD OUTTSR	MISC	O I
PLNTAP	g cm^{-2}	Scalar	Pesticide Applied to Crop Canopy	PESTAP OUTPST OUTTSR	PEST	O I I

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
PLVKRT	day^{-1}	Array	Foliage Pesticide Volatilization Rate	ECHO PLPEST PRZMRD	PEST	I I O
PNBRN	--	Array	Output Array for Time Series	OUTTSR		
PRECIP	cm	Scalar	Precipitation	PRZM HYDROL EROSN MASBAL OUTHYD OUTTSR	MET	O I I I I I
PTEMP	$g\ cm^{-3}$	Array	Temporary storage of total pesticide mass per cc water after advection step	MOC		M
PTITLE	--	Alpha-numeric	Comment Line to Input Information About Pesticide Parameters	PRZMRD ECHO	MISC	O I
PVFLUX	$g\ cm^{-2}\ day^{-1}$	Array	Daily Soil Pesticide Volatilization Flux	MASBAL OUTPST OUTRPT OUTTSR SLPST0 SLPST1	PEST	I I I I O O
PWIND	$m\ day^{-1}$	Array	Wind Velocity	PRZM		O
Q	m^3	Scalar	Runoff Volume	EROSN		
QC1	$cal\ cm^{-2}\ day^{-1}\ °K^{-1}$	Scalar	Sensible Heat Flux Term	SLTEMP		M
QEVF	$cal\ cm^{-2}\ day^{-1}$	Scalar	Evaporation Heat Flux	SLTEMP		M
QGHF	$cal\ cm^{-1}\ day^{-1}\ °K^{-1}$	Scalar	Soil Heat Flux Term	SLTEMP		M

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
QLW1	cal cm^{-2} day^{-1} $°K^{-4}$	Scalar	Atmospheric Longwave Radiation Component Term	SLTEMP		M
QLW2	cal cm^{-2} day^{-1} $°K^{-1}$	Scalar	Longwave Radiation Flux Term Emitted by Soil Surface	SLTEMP		M
QO	m^3/s	Scalar	Flow rate entering head of furrow	FURROW	IRGT	I
QQP	m^6 sec^{-1}	Scalar	Runoff Energy Factor	EROSN		
QS	m^3/s	Array	Flow rate in furrow at each downstream station	FURROW	IRGT	M
QSWR	cal cm^{-2} day^{-1}	Scalar	Net Shortwave Radiation Flux Term	SLTEMP		M
RATIO	--	Array	The ratio of point densities between adjacent horizons.	INITL MOC	HYDR	M
RETEAP	cm/hr	Scalar	Maximum rate of water that sprinklers can deliver	IRRIG	IRGT	I
RF	kg ha^{-1}	Scalar	Pesticide Runoff Flux	OUTPST		
RINUM	--	Scalar	Richardson Number	CANOPY		O
RMULT	--	Scalar	Multiplication Factor for Time Series Output	OUTTSR		
RMULT1	--	Scalar	Multiplication Factor for Curve Number AMC I	PRZMRD		
RMULT3	--	Scalar	Multiplication Factor for Curve Number AMC III	PRZMRD		
RNSUM	--	Scalar	Converts NSUM to a Real Number	EVPOTR		
RNUM	ha cm^{-2}	Scalar	Numerator of Peak Runoff Rate	EROSN		

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
RODPTH	--	Scalar	Number of Soil Compartments that Affect Runoff	HYDROL		
ROFLUX	g cm^{-2} day^{-1}	Scalar	Runoff Flux of Pesticide From Land Surface	SLPST0	PEST	O
				SLPST1		O
				MASBAL		I
				OUTHYD		I
				OUTTSR		I
RTR	day^{-1}	Array	Transformation Term from Daughter Product Consideration	PSTLNK	PEST	O
				SLPST0		I
				SLPST1		I
RUNOF	cm	Scalar	Current Runoff Depth	HYDROL	HYDR	O
				PRZM		I
				EROSN		I
				SLPST0		I
				SLPST1		I
				MASBAL		I
				OUTHYD		I
				OUTTSR		I
RVEL	--	Array	Retarded solute velocity	MOC		M
RZD	cm	Scalar	Maximum Root Zone Depth for All Crops	INITL		
				OUTHYD		
RZFLUX	g cm^{-2}	Scalar	Dispersive/Advective Flux of Pesticide Past the Bottom Root Zone Compartment	SLPST0	PEST	O
				SLPST1		O
				OUTTSR		I
RZI	--	Scalar	Active Root Zone Flag	INITL	MISC	O
				PLGROW		I
SA	kg ha^{-1}	Scalar	Application of Pesticide to the Soil	OUTPST		
SAIM	--	Scalar	Integrated Momentum Stability Parameter	CANOPY		O
SAND	percent	Array	Percent Sand in Each Soil Horizon	SLTEMP	HYDR	I

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
SD	kg ha^{-1}	Scalar	Sum of the Decay Fluxes From All Compartments in Soil Profile	OUTPST		
SDKFLX	g cm^{-2} day^{-1}	Scalar	Sum of the Decay fluxes From All Compartments in Soil Profile	SLPST0 SLPST1 OUTPST	PEST	O O I
SEDL	MTonne day^{-1}	Scalar	Erosion Sediment Loss	PRZM EROSN OUTHYD	HYDR	O M O
SF	Fraction	Scalar	Slope of furrow channel (vertical/horizontal)	FURROW	IRGT	I
SFAC	cm °C^{-1}	Scalar	Snowmelt Factor	PRZMRD ECHO HYDROL	MET	O I I
SIGMA0	--	Scalar	Summation Variable Used to Calculate K Factor in the Soil Thermal Conductivity Equation	SLTEMP		M
SIGMA1	cal cm^{-1} °C day^{-1}	Scalar	Total Numerator Value in the Soil Thermal Conductivity Equation	SLTEMP		M
SIGMA2	--	Scalar	Total Denominator Value in the Soil Thermal Conductivity Equation	SLTEMP		M
SJDAY	--	Scalar	Starting Day of Simulation	INITL		
SLKGHA	kg ha^{-1} day^{-1}	Scalar	Erosion Sediment Loss	EROSN		
SMDEF	cm	Scalar	Soil moisture deficit requiring irrigation	IRRIG	IRGT	O
SMELT	cm	Scalar	Current Daily Snowmelt Depth	HYDROL EROSN OUTHYD	HYDR	O

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
SNOW	cm	Scalar	Snowpack Accumulation Depth	SLTEMP	HYDR	I
SNOWFL	cm	Scalar	Current Snowfall Depth	HYDROL MASBAL OUTHYD OUTTSR	MET	O I I I
SOILAP	g cm^{-2}	Array	Pesticide Applied to the Soil	PESTAP PRZM OUTPST OUTTSR	PEST	O I I I
SOL	mole fraction mg l^{-1} umoles l^{-1}	Scalar	Pesticide Solubility - Karickhoff Model Kenaga Model Chiou Model	PRZMRD KDCALC		O I
SOLRAD	cal cm^{-2} day^{-1}	Scalar	Shortwave Solar Radiation	PRZMRD SLTEMP	MET	O I
SPESTR	g cm^{-3}	Array	Dissolved Pesticide in Each Soil Compartment	INITL PRZM PESTAP SLPST0 SLPST1	PEST	O I I I I
SPT	°C	Array	Temperature of Soil in Each Compartment	SLTEMP PRZM	MET	O I
SPTEMP	g cm^{-3}	Array	Temporary storage of dissolved pesticide mass per cc water after advection step	MOC SLPST1 INITL	PEST	M
SRC	g cm^{-3} day^{-1}	Array	Source Term from Daughter Product Consideration	PSTLNK SLPST0 SLPST1	PEST	O I I
SRCFLX	g cm^{-2} day^{-1}	Array	Source Flux of Pesticide from Each Soil Compartment	SLPST0 SLPST1 OUTPST	PEST	O O I

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
STEMP	°C	Array	Soil Compartment Temperature	KHCORR		I
STEP1	--	Alpha-numeric	Time Step of Water Output Summary	PRZMRD ECHO OUTHYD	MISC	O I I
STEP2	--	Alpha-numeric	Time Step of Pesticide Output Summary	PRZMRD ECHO OUTPST	MISC	O I I
STEP3	--	Alpha-numeric	Time Step of Concentration Profile Output Summary	PRZMRD ECHO OUTCNC	MISC	O I I
STITLE	--	Alpha-numeric	Comment Line to Input Information About Soil Parameters	PRZMRD ECHO	MISC	O I
STK	°K	Scalar	Soil Surface Temperature in Kelvin Scale	SLTEMP		M
STTDET	cm day^{-1}	Scalar	Daily Evaporation from the Top 5cm of Soil	SLTEMP EVPOTR	MET	I O
SU	kg ha^{-1}	Scalar	Sum of the Uptake Fluxes From All Soil Compartments	OUTPST		
SUMC	g	Array	Sum of mass in a compartment	MOC		M
SUMXP	kg ha^{-1}	Scalar	Sum of Soluble Pesticide in Profile	OUTPST		
SUPFLX	g cm^{-2} day^{-1}	Scalar	Sum of the Uptake Fluxes From All Soil Compartments	SLPST0 SLPST1 OUTPST OUTTSR	PEST	O O I I
SV	kg ha^{-1} day^{-1}	Scalar	Daily Soil Pesticide Volatilization Flux	OUTPST		O

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
SW	cm	Array	Current Water Depth in Each Soil Compartment	INITL HYDROL EVPOTR HYDR1 HYDR2 SLPST0 SLPST1 OUTTSR	HYDR	O I I I I I I I
T	--	Scalar	Fraction Compartment Check	INITL		
TA	day^{-1}	Array	Lower Diagonal Element of Tridiagonal Matrix	SLTEMP		M
TAPP	$g\ cm^{-2}$	Array	Total Pesticide Applied Per Application	PRZMRD ECHO INITL PESTAP	PEST	O I I I
TB	day^{-1}	Array	Diagonal Element of Tridiagonal Matrix	SLTEMP		M
TC	day^{-1}	Array	Upper Diagonal Element of Tridiagonal Matrix	SLTEMP		M
TCNC	$g\ cm^{-3}$	Array	Average Pesticide Concentration in Canopy	OUTPST		O
TCORR	mole cal^{-1}	Scalar	Temperature Correction Factor	KHCORR		M
TEMP	°C	Scalar	Ambient Air Temperature	SLTEMP	MET	I
TEMPK	°K	Scalar	Air Temperature in Kelvin Scale	SLTEMP		M
TEND	day	Scalar	Time required for point to move to compartment boundary	MOC		M
TERM	--	Scalar	Exponential Pesticide Washoff Term	PLPEST		

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
TERM1	--	Scalar	Exponential Pesticide Decay Term	PLPEST		
TERM2	--	Scalar	Product of Washoff and Decay Terms	PLPEST		
TF	°C	Array	Vector of Previous Time Step Soil Compartment Temperature	SLTEMP		M
TFRAC	--	Scalar	Total Fraction of Compartments Available for Evapotranspiration Extraction	EVPOTR		
THAIR	$cm^3\ cm^{-3}$	Array	Volumetric Air Content	SLPST0 SLPST1		O O
THCOND	$cal\ cm^{-1}\ day^{-1}\ °C^{-1}$	Array	Thermal Conductivity of Soil Compartment	SLTEMP		M
THEFC	$cm^3\ cm^{-3}$	Array	Field Capacity Water Content for Each Soil Horizon	SLTEMP	HYDR	I
THETAS	$cm^3\ cm^{-3}$	Array	Soil Compartment Water Content at Saturation	SLTEMP	HYDR	I
THETH	$cm^3\ cm^{-3}$	Scalar	Soil Moisture Content Half Way Between Wilting Point and Field Capacity in the Top Soil Compartments	INITL HYDROL	HYDR	O I
THETN	$cm^3\ cm^{-3}$	Array	Soil Water Content at the End of the Current Day for Each Soil Compartment	HYDR1 HYDR2 PRZM SLPST0 SLPST1 MASBAL OUTHYD OUTPST OUTTSR OUTCNC	HYDR	O O I I I I I I I I

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
THETO	$cm^3\ cm^{-3}$	Array	Soil Water Content at the End of the Previous Day for Each Soil Compartment	SLTEMP	HYDR	I
THEWP	$cm^3\ cm^{-3}$	Array	Wilting Point Water Content for Each Soil Horizon	SLTEMP	HYDR	I
THFLAG	--	Scalar	Soil Water Content Flag (0= Field Capacity and Wilting Point are Input, 1= Field Capacity and Wilting Point are Calculated)	PRZMRD ECHO PRZM	MISC	O I I
THKLY1	cm	Scalar	Thickness of Top Compartment	SLTEMP		
THKNS	cm	Array	Soil Horizon Thickness	PRZMRD ECHO INITL HYDROL	MISC	O I I I
THRUFL	cm	Scalar	Precipitation that Falls Past the Crop Canopy to the Soil Surface	HYDROL OUTHYD OUTTSR	MET	O I I
THZERO	$cal\ cm^{-1}\ day^{-1}\ {}^{o}C^{-1}$	Array	Thermal Conductivity of Soil at Water Content and Wilting Point	SLTEMP		M
TITLE	--	Alpha-numeric	Title of the Simulation (User Supplied)	PRZMRD ECHO	MISC	O I
TLEFT	day	Scalar	Travel time left in current time step	MOC		M
TMPK	°K	Scalar	Soil Temperature	KHCORR		M
TNDGS	day	Array	Total Number of Days in Each Growing Season	INITL PLGROW	CROP	O I
TOL	--	Scalar	Fraction Compartment Check	INITL		

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
TOP	--	Array	Location of top compartment in horizon where points are consolidated	INITL, MOC	HYDR	M
TOT	day m^{-1}	Scalar	Canopy Resistance	CANOPY		O
TOTAL	mg kg^{-1}	Array	Total Pesticide in Each Compartment	OUTCNC		
TOTR	day m^{-1}	Scalar	Total Canopy Resistance	CANOPY		O
TR	hr	Scalar	Duration of Average Erosive Storm Event	PRZMRD ECHO EROSN	MET	O I I
TRFLUX	g cm^{-2} day^{-1}	Array	Transformation Flux of Pesticide from Each Soil Compartment	SLPST0 SLPST1 OUTPST	PEST	O O I
TS	cm^3 cm^{-3}	Array	Previous Soil Compartment Water Content Minus Evapotranspiration	HYDR2		
TSRCFX	g cm^{-2} day^{-1}	Array	Sum of the Source Flux from All Compartments in Soil Profile	SLPST0 SLPST1 OUTPST	PEST	O O I
TSW	cm	Scalar	Total Soil Water in Compartments Available for Evapotranspiration Extraction	EVPOTR		
TTHKNS	cm	Scalar	Total Thickness of Soil Profile (For Computational Check)	INITL		
TTRFLX	g cm^{-2} day^{-1}	Array	Sum of the Transformation Flux from All Compartments in Soil Profile	SLPST0 SLPST1 OUTPST	PEST	O O I
TWLVL	cm cm^{-1}	Scalar	Fraction of Water to Soil Depth for Runoff Calculation	HYDROL		

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
TWP	cm	Scalar	Total Wilting Point Depth in Compartments Available for Evapotranspiration Extraction	EVPOTR		
U	--	Array	Upper Decomposed Matrix	TRDIAG		
UBT	°C	Scalar	Upper Boundary or Soil Surface Temperature	SLTEMP		M
UPF	kg ha^{-1}	Scalar	Daily Pesticide Uptake Flux in Profile	OUTPST		
UPFLUX	g cm^{-2}	Array	Uptake Flux of Pesticide From Each Soil Compartment	SLPST0 SLPST1 OUTPST	PEST	O O I
UPTKF	--	Scalar	Plant Pesticide Uptake Efficiency Factor	PRZMRD ECHO PLGROW	PEST	O I I
URH	m day^{-1}	Scalar	Wind Velocity at Reference Height	CANOPY PRZM		I O
USLEC	--	Array	Universal Soil Loss Equation 'C' Factor	PRZMRD ECHO EROSN	HYDR	O I I
USLEK	--	Scalar	Universal Soil Loss Equation 'K' Factor	PRZMRD ECHO EROSN	HYDR	O I I
USLELS	--	Scalar	Universal Soil Loss Equation 'Ls' Factor	PRZMRD ECHO EROSN	HYDR	O I I
USLEP	--	Scalar	Universal Soil Loss Equation 'P' Factor	PRZMRD ECHO EROSN	HYDR	O I I
USTAR	m day^{-1}	Scalar	Friction Velocity	CANOPY		O
UTEMP	°C	Array	Air Temperature	CANOPY		I

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
UWIND	m day^{-1}	Array	Wind Velocity	CANOPY		I
VAPLMD	cal cm^{-1} day^{-1} $°C^{-1}$	Scalar	Thermal Conductivity of Vapor in the Soil Pores	SLTEMP		
VAR1	kg ha^{-1}	Scalar	Daily Advection/Dispersion Flux of Pesticide Into a Compartment	OUTPST		
VAR2	kg ha^{-1}	Scalar	Daily Advection/Dispersion Flux of Pesticide Out of a Compartment	OUTPST		
VAR2D	cm	Scalar	Water Storage in a Single Compartment for the Previous Day	OUTHYD		
VAR2M	cm	Scalar	Water Storage in a Single Compartment for the Previous Month	OUTHYD		
VAR2RZ	kg ha^{-1}	Scalar	Daily Advection/Dispersion Flux of Pesticide Out of the Root Zone	OUTPST		
VAR2Y	cm	Scalar	Water Storage in a Single Compartment for the Previous Year	OUTHYD		
VAR3	kg ha^{-1}	Scalar	Pesticide Storage in a Single Compartment for the Previous Day	OUTPST		
VEL	cm day^{-1}	Array	Water Velocity in Each Soil Compartment	HYDR1 HYDR2 SLPST0 SLPST1	HYDR	O O I I
VHTCAP	cal cm^{-3} $°C^{-1}$	Array	Heat Capacity Per Unit Volume of Soil	SLTEMP		M

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
VLFLAG	--	Scalar	Advection flux flag (0 = all soil water velocities are zero, 1 = soil water velocity is nonzero)	HYDR1 PRZM HYDR2	HYDR	I
VOLCOR	--	Scalar	A Variable Used to Convert Weight Percents of Soil Constituents to Volume Fractions of Bulk Volume	SLTEMP		
WBAL	cm	Scalar	Current Water Balance Error	MASBAL OUTHYD	HYDR	O I
WEIGHT	kg m^{-2}	Scalar	Current Plant Dry Foliage Weight	PLGROW PESTAP	CROP	O I
WF	kg ha^{-1}	Scalar	Daily Pesticide Washoff Flux	OUTPST		
WFMAX	kg m^{-2}	Array	Maximum Plant Dry Foliage Weight at Full Canopy	PRZMRD ECHO INITL	CROP	O I I
WIND	cm sec^{-1}	Scalar	Wind Speed	PRZMRD SLTEMP PRZM	MET	O I I
WLVL	cm	Scalar	Total Soil Water in the Compartments that Affect Runoff	HYDROL		
WOFLUX	g cm^{-2} day^{-1}	Scalar	Washoff Flux of Pesticide From Plant Foliage	SLPST0 SLPST1 OUPPST	PEST	O O I
WP	cm	Array	Wilting Point Water Depth in a Soil Compartment	HYDR EVPOTR	O	
WPV	--	Array	Regression Coefficients for Prediction of Wilting Point Soil Water Content	THCALC		

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
WTERM	g cm^{-2}	Scalar	Current Daily Pesticide Washoff Loss	PLPEST	PEST	O
				SLPST0		I
				SLPST1		I
X	g cm^{-3}	Array	Dissolved Pesticide in Each Soil Compartment	TRDIAG	PEST	
				SLPST0	PEST	O
				SLPST1		O
				MASBAL		I
				OUTPST		I
				OUTTSR		I
				OUTCNC		I
				PRZM		I
XFRAC	Fraction	Scalar	Location in furrow where infiltration is to be used in PRZM transport calculations (as fraction of total furrow length)	IRRIG	IRGT	I
XL	m	Scalar	Length of furrows	IRRIG	IRGT	I
				FURROW		I
						O
XP	g cm^{-3}	Array	Total Pesticide in Each Soil Compartment	MASBAL		
XVOL	fraction	Array	Volume Fraction of Soil Constituent	SLTEMP		
Y	--	Array	Intermediate Matrix Solution Array	TRDIAG		
YDOUT	kg ha^{-1}	Array	Annual Pesticide Decay From Each Soil Compartment	OUTPST	ACCUM	M
YEAR	--	Alpha-numeric	Flag for Annual Water and Pesticide Summary Output	PRZM		
YEOUTW	cm	Array	Annual Evapotranspiration From Each Soil Compartment	OUTHYD	ACCUM	M
YINPP	kg ha^{-1}	Array	Annual Advective/Dispersive Flux Into Each Soil Compartment	OUTPST	ACCUM	M

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
YINPP1	kg ha^{-1}	Scalar	Annual Pesticide Applied to Foliage	OUTPST	ACCUM	M
YINPP2	kg ha^{-1}	Scalar	Annual Pesticide Applied to Soil	OUTPST	ACCUM	M
YINPW	cm	Array	Annual Infiltration Into Each Soil Compartment	OUTHYD	ACCUM	M
YINPW1	cm	Scalar	Annual Precipitation	OUTHYD	ACCUM	M
YINPW2	cm	Scalar	Annual Snowfall	OUTHYD	ACCUM	M
YOUTP	kg ha^{-1}	Array	Annual Pesticide Uptake From Each Soil Compartment	OUTPST	ACCUM	M
YOUTP1	kg ha^{-1}	Scalar	Annual Pesticide Washoff Flux	OUTPST	ACCUM	M
YOUTP2	kg ha^{-1}	Scalar	Annual Pesticide Runoff Flux	OUTPST	ACCUM	M
YOUTP3	kg ha^{-1}	Scalar	Annual Pesticide Erosion Flux	OUTPST	ACCUM	M
YOUTP4	kg ha^{-1}	Scalar	Annual Foliar Pesticide Decay Flux	OUTPST OUTPST	ACCUM ACCUM	M M
YOUTP5	kg ha^{-1}	Scalar	Total Annual Pesticide Uptake Flux	OUTPST	ACCUM	M
YOUTP6	kg ha^{-1}	Scalar	Total Annual Pesticide Soil Decay Flux	OUTPST	ACCUM	M
YOUTW	cm	Array	Annual Exfiltration From Compartment	OUTHYD	ACCUM	M
YOUTW1	cm	Scalar	Annual Canopy Evaporation	OUTHYD	ACCUM	M
YOUTW2	cm	Scalar	Annual Trufall	OUTHYD	ACCUM	M
YOUTW3	cm	Scalar	Annual Runoff	OUTHYD	ACCUM	M
YOUTW4	cm	Scalar	Annual Snowmelt	OUTHYD	ACCUM	M

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
YOUTW5	cm	Scalar	Total Annual Evapotranspiration	OUTHYD	ACCUM	M
YOUTW6	MTonne	Scalar	Total Annual Sediment Loss	OUTHYD	ACCUM	M
YSTR	cm	Array	Previous Year Storage of Water in Each Soil Compartment	OUTHYD OUTHYD	ACCUM ACCUM	M M
YSTR1	cm	Scalar	Annual Canopy Interception	OUTHYD	ACCUM	M
YSTR2	cm	Scalar	Annual Snow Accumulation	OUTHYD	ACCUM	M
YSTRP	kg ha^{-1}	Array	Storage of Pesticide From Previous Year in Each Soil Compartment	OUTPST	ACCUM	M
YSTRP1	kg ha^{-1}	Scalar	Storage of Foliar Pesticide	OUTPST	ACCUM	M
Z	Fraction	Scalar	Side slope of furrow channel walls (horizontal/vertical)	FURROW	IRGT	I
Z	--	Array	Location of moving points	MOC INITL	HYDR	M
ZC	--	Array	Location of fixed compartment center	MOC INITL	HYDR	M
ZCH PRZM	m	Scalar O	Canopy Height	CANOPY		I
				SLTEMP		M
ZCTOT	--	Scalar	Concentration weighted locations of consolidated points	MOC	-	M
ZIN	--	Array	Temporary storage of new point locations	MOC		M
ZO	m	Scalar	Roughness Height	CANOPY SLTEMP		O M

Table 8-3. PRZM PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (concluded)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ZRH	m	Scalar	Reference Height	CANOPY PRZM		I O
ZTOT	--	Scalar	Location of consolidated Points	MOC	-	M
ZWIND	m	Scalar	Distance Above the Ground Where Wind Speed was Measured	PRZMRD PRZM SLTEMP		O O I

Table 8-4. VADOFT PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATIONS

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
A	--	ARRAY	Left Diagonal of a Tridiagonal Matrix	ASSEMF ASSEMT	ASOLV	M
ASTORN	--	SCALAR	Value of A(NP) Where NP=Number of Nodes	ASSEMF ASSEMT BALCHK	WORKA	M
B	--	ARRAY	Main Diagonal of a Tridiagonal Matrix	ASSEMF ASSEMT	ASOLV	M
BALSTO	--	ARRAY	Array Containing Mass Balance Information	VADINP BALCHK		M O
BSTOR1	--	SCALAR	Value of B(1)	ASSEMF ASSEMT BALCHK	WORKA	M
BSTORN	--	SCALAR	Value of B(NP) Where NP=Number of Nodes	ASSEMF ASSEMT BALCHK	WORKA	M
C	--	ARRAY	Right Diagonal of a Tridiagonal Matrix	ASSEMF ASSEMT	ASOLV	M
CORD	L	ARRAY	Nodal Coordinates	VADINP VSWCOM	ADISC	I
CSTOR1	--	SCALAR	Value of C(1)	ASSEMF ASSEMT BALCHK	WORKA	M
CTRFAC	--	ARRAY	Coordinate Transformation Factors for Different Soil Materials	CONVER DSWFUN VADINP	WORKN	M
D	--	ARRAY	Right-Hand-Side Vector of a Tridiagonal Matrix	ASSEMF ASSEMT	ASOLV	M
DETAND	-	ARRAY	Nodal Storage Factor	ASSEMF	WELEM	M

Table 8-4. VADOFT PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATIONS (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
DIS	L M/L**3	ARRAY	Current Nodal Value of Head of Concentration	VADINP ASSEMF BALCHK VARCAL VSWCOM	BSOLV	M O
DLAMDA	1/t	SCALAR	Value of Decay Constant for the Node Currently Being Evaluated	VADINP ASSEMT VARCAL	CONTR	M
DLAMND	1/t	SCALAR	Nodal Value of Decay Constant	VADINP ASSEMT BALCHK VARCAL	VVELEM	I
DPKND	L/t	ARRAY	Nodal Values of Hyd. Conductivity Increment	ASSEMF	WELEM	M
DPKRAV	L**2	SCALAR	Value of Rel. Perm. for Node Currently Being Solved	ASSEMF PKWFUN		M
DSTOR1	--	SCALAR	The Value of D(1)	ASSEMF ASSEMT BALCHK	WORKA	M
DSTORN	--	SCALAR	The Value of D(NP) Where NP = Number of Nodes	ASSEMF ASSEMT BALCHK	WORKA	M
DTEPS	--	SCALAR	Time Step Tolerance Parameter	VADINP		M
DTMARK	--	SCALAR	Marker Time Increment	VADINP		M
DX	--	SCALAR	DX = THL(I) NEL	VADINP		M
EL	L	SCALAR	Elemental Values for Finite-Element Element Length Formulation	VADINP ASSEMF ASSEMT BALCHK VARCAL VSWCOM	VVELEM	M

Table 8-4. VADOFT PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATIONS (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ETAND	--	ARRAY	Nodal Values of Fluid Storage Factor	ASSEMF ASSEMT BALCHK	WELEM	M
FLX1	L**3/t	SCALAR	Value of Fluid Flux Entering Node 1 (for Flow FLX1 = 0.0)	VADINP ASSEMT HFINTP VARCAL	CONTR	M
FLXN	L**3/t	SCALAR	Value of Fluid Flux Entering the Last Node (for Flow FLX1 = 0.0)	VADINP ASSEMT HFINTP VARCAL	CONTR	M
FVAL	-	ARRAY	Functional Coefficient Values for the Soil Moisture Relationship	VADINP ASSEMT HFINTP SWFUN CONVER DSWFUN	MDATA	M
HAVE	L	SCALAR	Average Head Value	ASSEMF SWFUN DSWFUN		M
HCAP	L	ARRAY	Value of Pressure Head on Press. Head vs. Sat. Curve	VADINP ASSEMF INTERP	SWHDA	M
HCRIT	L	SCALAR	Critical Head Value	ASSEMF SWFUN DSWFUN		I
HDOBS	L M/L**3	ARRAY	Head or Concentration of Observation Node for Current Time	VADINP	DAOBS	M O
HINV	L M/L**3	SCALAR	Default Value of Initial Head or Concentration	VADINP		I
HTOL	L	SCALAR	Head Tolerance Allowed for Nonlinear Solution	VADINP ASSEMF VARCAL DSWFUN	CONTR	I

Table 8-4. VADOFT PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATIONS (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
HVTM	L	ARRAY	Value of function corresponding to Time Values(TMHV)	VADINP HFINTP		M
IBTND1	--	SCALAR	Last Node Boundary Condition Code (1=1st type, 0=3rd type)	VADINP ASSEMF ASSEMT VARCAL		I
IBTNDN	__	SCALAR	Last Node Boundary Condition Code (1=1st Type, 0=3rd type)	ASSEMF VADINP ASSEMT VARCAL		I
ICONVG	--	SCALAR	Convergence Flag (1=Converged, 0=Not Converged)	VADINP VARCAL		I
IHORIZ	--	SCALAR	Simulation Orientation Indicator (0=Vertical, 1=Horizontal)	VADINP		I
IKALL	--	SCALAR	Time Stepping Scheme Indicator (1=Backward, 0=Central)	VADINP		I
ILAYR	--	SCALAR	Current Layer Number	VADINP		I
IMAT	--	SCALAR	Counter Used in Looping with Respect to Materials	VADINP ASSEMF ASSEMT INTERP PKWFUN SWFUN CONVER DSWFUN		I
IMATL	--	ARRAY	Material Identifing Number for Current Layer	VADINP		I
IMBAL	--	SCALAR	Mass Balance Computation Indicating Parameter	VADINP	CONTR	I

Table 8-4. VADOFT PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATIONS (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
IMOD	--	SCALAR	For Modified Newton Raphson Solution Procedure	VADINP DSWFUN	CONTR1	I
IMODL	--	SCALAR	Simulation Identifier (Flow or Transport)	VADINP BALCHK VARCAL	CONTR	I
INEWT	--	SCALAR	Nonlinear Iterative Procedure Flag (1=Newton, 0=Picard, 2=Modified N-R)	VADINP ASSEMF VARCAL	CONTR	I
INOCTS	--	SCALAR	Number of Computation Time Steps Required to Simulate This Target Time Step	VADINP VARCAL		I
INPFL	--	SCALAR	Unit Number for Input File	VADINP		I
INTSPC	--	SCALAR	Initial Condition Specifier for Head Conversion Convert Initial Head Values (1=Yes, 0=No)	VADINP		I
IOBSND	--	SCALAR	Observation Node Index	WORKA		I
IPRCHK	--	SCALAR	Print Check Flag (Triggers Additional Diagnostic Output)	VADINP ASSEMF ASSEMT BALCHK VARCAL CONVER		I
IPROP	--	ARRAY	Generated Material Property Identifiers	VADINP ASSEMF ASSEMT	MDATA	I
IREP	--	SCALAR	Time Step Refinement Counter	VADINP VARCAL		M

Table 8-4. VADOFT PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATIONS (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
IREPMX	--	SCALAR	Maximum Number of Nonlinear Solution Cycles	VADINP VARCAL		I
IRESOL	--	SCALAR	Maximum Number of Time Step Refinements	VADINP VARCAL		I
IRLTYP	--	SCALAR	Flag for the Type of Relative Function Being Evaluated	ASSEMF INTERP		I
ITCND1	--	SCALAR	Node 1 Boundary Condition Flag (1 = Transient, 0 = Steady State)	VADINP HFINTP	VVELEM	I
ITCNDN	--	SCALAR	Node 1 Boundary Condition Flag (1 = Transient, 0 = Steady State)	VADINP HFINTP	VVELEM	I
ITER	--	SCALAR	Iterative Counter (Current Iteration Number)	VADINP ASSEMF ASSEMT BALCHK VARCAL VSWCOM		M
ITMARK	--	SCALAR	Backup File Output Indicator	VADINP VSWCOM		M
ITMFC	--	SCALAR	Marker Time Increasing Parameter	VADINP VSWCOM		M
ITMGEN	--	SCALAR	Marker Time Value Generation Indicator	VADINP		I
ITRANS	--	SCALAR	Transient Steady-State Flag (1=TR, 0=SS)	VADINP ASSEMF VARCAL	CONTR	I
ITSGN	--	SCALAR	Time Step Generation Indicator	VADINP		I

Table 8-4. VADOFT PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATIONS (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ITSTH	--	ARRAY	Identifies Location of Previous Time Value of Time Graph	VADINP HFINTP		I
IVSTED	--	SCALAR	Steady-State Velocity Field Indicator	VADINP		I
KPROP	--	SCALAR	Flag for Perm-Saturation and Pressure Head-Saturation Curves (1-Functional, 0-Tabulated)	VADINP ASSEMF VARCAL	CONTR	I
MARK	--	SCALAR	Flow Direction Flag (1-Vertical, 0-Horizontal)	VADINP ASSEMF VARCAL VSWCOM	CONTR	I
MM	--	SCALAR	Place Holder for Loop Incrementer			M
MXMAT	--	SCALAR	Maximum Number of Materials Allowed (Due to the Size of Arrays)	VADINP ASSEMF ASSEMT INTERP PKWFUN SWFUN DSWFUN		I
MXNODE	--	SCALAR	Maximum Number of Nodes Allowed (Due to the Size of Some Arrays)	VADINP ASSEMF ASSEMT BALCHK TRIDIV VARCAL VSWCOM		I
MXTMV	t	SCALAR	Maximum Time Value to be Interpolated	VADINP HFINTP		I
NDCOUN	--	SCALAR	Material Number Temporary Counter	VADINP		M

Table 8-4. VADOFT PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATIONS (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NDM1	--	SCALAR	Counter Minus One NDM1 = NDCOUN	VADINP		M
NDOBS	--	ARRAY	Nodal Values of Observation Nodes	VADINP	DAOBS	I
NE	--	SCALAR	Number of Elements in the Linear Representation	VADINP VSWCOM	CONTR	I
NEL	--	SCALAR	Storage Location for the Number of Finite Elements in the Current Layer NELM(I)	VADINP		M
NELM	--	ARRAY	Number of Finite Elements in the Current Layer	VADINP		I
NITMAX	--	SCALAR	Maximum Number of Nonlinear Iterations Allowed per Time Step	VADINP VARCAL	CONTR	I
NLAYRG	--	SCALAR	Number of Layers That Need to be Descritized	VADINP		I
NMAT	--	SCALAR	Number of Soil Materials	VADINP CONVER		I
NOBSND	--	SCALAR	Number of Observation Nodes in the Simulation	VADINP		I
NONU	--	SCALAR	Nonuniform Initial Condition Indicator	VADINP		I
NOWRIT	--	SCALAR	Restart Data Writing Indicator	VADINP		I
NP	--	SCALAR	Total Number of Nodal Points	VADINP ASSEMF ASSEMT BALCHK TRIDIV VARCAL VSWCOM	CONTR	I

Table 8-4. VADOFT PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATIONS (continued)

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
NPIN	--	SCALAR	Number of Nondefault Initial Values	VADINP		I
NPROB	--	SCALAR	Number of Simulations to be Made	VADINP		I
NSTEP	--	SCALAR	Nodal Value Printout Control Parameter	VADINP BALCHK	CONTR	I
NTN1	--	SCALAR	Storage Location for NTSNDH(1)	VADINP		M
NTNP	--	SCALAR	Storage Location for NTSNDH(NP)	VADINP		M
NTOMT	--	SCALAR	Number of Backup File Output Marker Time Values	VADINP VSWCOM		I
NTS	--	SCALAR	Number of Time Steps in This Simulation	VADINP		M
NTSNDH	--	ARRAY	Number of Time Values on the Time Graph ([1]=CONC, [2]=HEAD)	VADINP HFINTP		I
NUMK	--	ARRAY	Values of Permeability from the Permeability vs Saturation Table for Each Material	VADINP ASSEMF INTERP	SWHDA	I
NUMP	--	ARRAY	Number of Pressure Head vs. Saturation Values for Each Material	VADINP ASSEMF INTERP	SWHDA	I
NUMT	--	SCALAR	Time Step Incrementor	VADINP		I
NVPR	--	SCALAR	Velocity Printout Control Parameter	VADINP VSWCOM	CONTR	I
NVREAD	--	SCALAR	Velocity Reading Indicator	VADINP		I

Table 8-4. VADOFT PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATIONS (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
OUTFL	--	SCALAR	Output File Unit Number	VADINP ASSEMF ASSEMT BALCHK INTERP VARCAL VSWCOM		I
PCUR	L M/L**3	ARRAY	Current Value of Pressure Head or Concentration for the Current Time Step	ASSEMF VARCAL	BSOLV	M
PINT	L M/L**3	ARRAY	Initial Value of Pressure Head or Concentration	VADINP ASSEMF ASSEMT BALCHK VARCAL	BSOLV	I
PKND	L/t	ARRAY	Nodal Values of Hydraulic Conductivity	VADINP ASSEMF VSWCOM	WELEM	M
PKRW	L**2	ARRAY	Value of Relative Permeability (on Perm. vs. Sat. Curve)	VADINP ASSEMF INTERP	SWHDA	M
PKWOUT	L**2	SCALAR	Relative Permeability Computed Using Function Then Passed Back	PKWFUN		M
PROP		ARRAY	Saturated Material Properties (Flow or Transport) Flow-Hydraulic Conductivity Porosity, Specific Storage Air Entry Pressure Transport-Dispersivity, Porosity, Retardation Diffusion	VADINP ASSEMF ASSEMT	MDATA	I
QVTM	L**3/t	ARRAY	Volumetric Water Flux Values Corresponding to Time Values	VADINP HFINTP		M

Table 8-4. VADOFT PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATIONS (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
SLOPE	--	SCALAR	Slope of the Line Between the Points Being Interpolated	HFINTP INTERP		M
SSWV	--	ARRAY	Value of Water Phase Saturation (on Press. Head vs Sat. Curve)	ASSEMF INTERP	SWHDA	M
STMARK	t	SCALAR	Starting Marker Time Value	VADINP		M
SWAVE	--	SCALAR	Average Water Saturation	ASSEMF PKWFUN		M
SWDFI	--	ARRAY	Default Value of Water Saturation for the Current Material	VADINP		I
SWND	--	ARRAY	Current Water Saturation at the Node Being Evaluated	VADINP ASSEMF ASSEMT VARCAL VSWCOM	VVELEM	M
SWNDPT	--	ARRAY	Water Saturation for the Node at Previous Time Step	VADINP VSWCOM	VVELEM	M
SWRKP	--	ARRAY	Temporary Working Array	CONVER	WORKN	M
SWV	--	ARRAY	Value of Water Phase Saturation (on Perm. vs. Sat. Curve)	VADINP ASSEMF INTERP	SWHDA	M
TAP8	--	SCALAR	Unit Number for Restart File	VADINP		I
TAP10	--	SCALAR	Unit Number of Flow-to-Transport File (Darcy Vel. & Water Sat.)	VADINP VSWCOM	MDATA	I
TDIFF	t		TDIFF=TMCUR-TMVECX	VADINP		M

Table 8-4. VADOFT PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATIONS (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
TERIFL	--	SCALAR	Unit Number for Input File	VADINP		I
TEROFL	--	SCALAR	Unit Number for Output File	VADINP		I
TFAC	--	SCALAR	Time Step Multiplier	VADINP		I
THETA	--	SCALAR	Value Used in the Time Stepping Scheme (Theta=0.5 for Central Difference Scheme, Theta=1.0 for Backward Difference Scheme)	VADINP ASSEMT BALCHK VARCAL		M
THETM1	--	SCALAR	Theta Minus One	VADINP ASSEMT BALCHK VARCAL		M
THL	L	ARRAY	Thickness of Current Layer	VADINP		M
TIN	t	SCALAR	Value of Initial Time Step	VADINP ASSEMF ASSEMT BALCHK VARCAL	CONTR	I
TIMA	t	SCALAR	Initial Time Value of the Simulation	VADINP VSWCOM	CONTR	I
TIMAKP	t	SCALAR	Storage Location for the Value of Time Where Iteration Computation is Taking Place	VADINP		M I
TITLE	--	ALPHA-NUMERIC ARRAY	Title of Simulation	VADINP		I
TMACCU	L**3 M	SCALAR	Quantitative Storage Water Volume or Solute Mass	VADINP BALCHK	CONTR	M

Table 8-4. VADOFT PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATIONS (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
TMAX	t	SCALAR	Maximum Time Step Size	VADINP		I
TMCUR	t	SCALAR	Current Time Value	VADINP VSWCOM		M
TMDCAY	M	SCALAR	Cumulative Solute Mass Decay	VADINP BALCHK	CONTR	M
TMFOMT	t	ARRAY	Time Values for Output to the Backup File	VADINP VSWCOM	ADISC	I
TMHV	t	ARRAY	Time Values at the Interpolation Points ([1]=CONC, [2]=HEAD)	VADINP HFINTP		M
TMVEC	t	ARRAY	Values of Time Generated by the Code, to be Used in the Simulation	VADINP BALCHK	ADISC	I M
TMVECX	t	SCALAR	Extra Time Value Due to the Reduction of a Time Step When Solution is not Converging	VADINP BALCHK HFINTP VARCAL		M
UWF	--	SCALAR	Value of Upstream Weighting Factor for the Node Currently Being Evaluated	VADINP ASSEMT VARCAL	CONTR	M
UWFI	--	ARRAY	Value of Upstream-Weighting Factor for the Current Material	VADINP		M
VALND1	--	SCALAR	Value of First Node (Depending on: Type of Run & Type of Boundary	VADINP ASSEMF ASSEMT HFINTP VARCAL		M
VALNDN	--	SCALAR	Value of Last Node (Depending on: Type of Run & Type of Boundary	VADINP ASSEMF ASSEMT HFINTP VARCAL		M

Table 8-4. VADOFT PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATIONS (concluded)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
VDAR	L/t	ARRAY	Darcy Velocity for Each Node	VADINP ASSEMF BALCHK VARCAL VSWCOM	VVELEM	M O
VDARPT	L/t	ARRAY	Nodal Darcy Velocities at Previous Time	VADINP VSWCOM	VVELEM	M
VDFI	L/t	ARRAY	Default Value of Darcy Velocity for Current Material	VADINP		I
XX	--	SCALAR	The X value Passed in INTERP (to be Used in the Interpolation)	INTERP		M
YY	--	SCALAR	The Y Value Passed in INTERP (to be Used in the Interpolation	INTERP		M

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
A	--	Array	Left Diagonal of Tridiagonal Matrix	TRIMOD	TRIDIA	M
AA	--	Array	Element Coefficient Matrix	ASSEMV	ELSTOR	
				EBFOR1		M,O
				EBFOR2		M,O
AI1	--	Array	Element Right Hand Side Vector	ASSEMV	ELSTOR	
				BALCHS		M
				EBFOR1		M,O
				EBFOR2		M,O
AK	--	Array	Global Coefficient Matrix	ASSEMV	WAVE1	M
				MATMOD		M
				SOLVEC		M
				SOLVEP		M
ALPHAL	--	Scalar	Longitudinal Dispersivity	ASSEMV		M
ANODE	L**2	Array	Nodal Areas	SMIOIN	NDSTOR	
				ANDCAL		M
				BALCHS		
				MATMOD		
AR	--	Array	Right-Hand Side Vector of Tridiagonal System	CPCAL	TRIDIA	M,O
ATPROP	Report	Array	Aquitard Properties	SMIOIN	MDATAT	I
				CPCAL		
B	--	Array	Central Diagonal of Tridiagonal Matrix	TRIMOD		
BR	--	Array	Working Array for Formulation of Tridiagonal System	SMIOIN	TRIDIA	M
				CPCAL		M,O
C	--	Array	Right Diagonal of Tridiagonal Matrix	TRIMOD		M
CC	M	Array	Element Mass Storage Matrix	BALCHS	ELSTOR	M
				EBFOR1		M,O
				EBFOR2		M,O

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
CD	M	Array	Element Mass Decay Matrix	BALCHS	ELSTOR	M
				EBFOR2		M,O
CON	M/L**3	Array	Nodal Values of Concentration In Aquitard Column	CPCAL	TRIDIA	O
CONVND	L/t	ARRAY	Nodal Value of Vertical Conductivity	SMIOIN	NDSTOS	M
				MATMOD		
CORD	--	Array	Nodal Coordinates	SMIOIN	MSHDAT	M,O
				FILPLT		
				FILPRW		O
				MESHGN		M
CR	--	Array	Working Array for the Formulation of the Tridiagonal System	CPCAL	TRIDIA	M,O
CTEMP	--	Array	Temporary Working Array	BALCHS	WORKS	M
D	--	Array	Right-Hand Side Vector of Tridiagonal System	TRIMOD		
DAKP	L**2	Array	Element Nodal Area	SMIOIN	ESTORE	M
				EBFOR1		O
				EBFOR2		
DEMND	L**3/t	Array	Nodal Values of Vertical Leakage Coefficient	SMIOIN	NDSTOS	M
				MATMOD		
DIS	L M/L**3	Array	Current Nodal Values of the Dependent Variable (Head/Conc.)	SMIOIN	WAVE	M
				BALCHS		
				CPCAL		
				EBFOR1		
				EBFOR2		
				FILHED		
				FILPLT		
				FILPRW		O
				MATMOD		O
				PBC		M
				QCAL		
				THUPDT		M
				VARCAL		M
				VELCOM		

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
DIST	--	Array	Dimensionless Nodal Coordinate for an Aquitard Column	SMIOIN CPCAL	VDISC	I,M,O M
DLAM	1/t	Array	Aquifer Decay Coefficient	SMIOIN	RDATA	I,O
DLEL	1/t	Array	Elemental Value of Aquifer Decay Coefficient	SMIOIN EBFOR2	RDATA	M
DPCOL	1/t	Array	Default Value of the Decay Coefficient of an Aquitard Column	SMIOIN CPCA	RDATA	M
DX	L	Scalar	Nodal Spacing of First Grid Block Nodal Spacing in the X-Direction	SMIOIN CPCAL DXYGEN MESHGEN		I,O M M
DYMAX	L	Scalar	Maximum Allowable Value of Nodal Spacing	SMIOIN DXYGEN MESHGEN		I,O
DXV	L	Array	Vertical Spacing of the Nodes in the Aquitard Column	CPCAL	VDISC	M
DY	L		Nodal Spacing in the Y-Direction	SMIOIN MESHGN		I,O
EI1	--	Array	Element Right Hand Side Vector	BALCHS	ELSTOR	M
EL	L	Scalar	Length of a Particular Rectangular Element	EBFOR1 EBFOR2 VELCOM	ESTORE	M M M M
ELKP	L	Array	Lengths of All Rectangular Elements in the Grid	SMIOIN ANDCAL EBFOR1 EBFOR2 VELCOM	ESTORE	M

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
EM	L	Array	Width of a Particular Rectangular Element	EBFOR1		M
				EBFOR2		M
				VELCOM		M
						M
EMKP	L	Array	Widths of All Rectangular Elements in the Grid	SMIOIN	ESTORE	M
				ANDCAL		
				EBFOR1		
				EBFOR2		
				VELCOM		
ETA	--	Scalar	Back Substitution Parameter	CPCAL		
				TRIMOD		M
ETAKP	--	Array	Back Substitution Parameter of All Aquitard Columns	SMIOIN	VDISC	
				BALCHS		
				CPCAL		M,O
				MATMOD		M,O
FIZ1	--	Array	Working Element Right Hand Side Vector	ASSEMV	ELSTOR	
				EBFOR1		M
FLUXV	L**3/t M/t	Array	Current Values of Prescribed Nodal (Fluid/Solute) Fluxes	BUPDAT	FDATA	M
				HFINTP		M
				PBC		M
FLUXVO	L**3/t M/t	Array	Default Steady-State values of Prescribed Nodal (Fluid/Solute) Fluxes	SMIOIN	FDATA	I
				BUPDAT		
FNDSTO	--	Array	Array Containing Mass Balance Information	BALCHS	WORKS	M,O
FVAL	--	Array	Working Arrays of Nodal Values	ASSEMV	ABOUN	
				PBC		M
FVTM	L**3/t	Array	Prescribed Nodal Fluxes at Various Times	SMIOIN	BCDATA	I,O
				HFINTP		
GAMKP	L**3/t	Array	Values of Vertical Leakage Fluxes for Various Aquitard Columns	CPCAL	VDISC	M

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
GAMMA	L**3	Scalar	Value of Vertical Leakage Flux for Particular Aquitard Column	CPCAL TRIMOD	TRIDIA	M,O M
GDECAY	1/t	Array	Nodal Values of Solute Mass Decay Rates	BALCHS	WORKS	M
GMZ	--	Array	Nodal Storage Array	ASSEMV BALCHS FILVEL	ESTORE	M M
HDOBS	L M/L**3	Array	Values (Head/Conc.) at Specified Observation Nodes	SMIOIN VARCAL	BNDOUT	O M
HDTEL		Array	Element Bookkeeping Array	EBFOR1	ELSTOR	M
HIAQFR	L M/L**3	Array	Initial Values of the Dependent Variable (Head/Conc.) in Aquifers	SMIOIN	INTDAT	I
HICOL	L M/L**3	Array	Overriding Initial Values (Head/Conc.) in Aquitard Columns	SMIOIN CPCAL	INTDAT	I,M,O
HINT	L M/L**3	Array	Nodal Values (Head/Conc.) in Aquifers At Previous Time Levels	SMIOIN BALCHS EBFOR1 EBFOR2 FILHED FILPRW MATMOD		I,M,O M
HPATD	L M/L**3	Array	Current Values (Head/Conc.) in the Aquitard	SMIOIN CPCAL FILHED FILPRW	WORKM	M M,O O
HSTORE	L M/L**3	Array	Array Containing Temporary Values (Head/Conc.) at the Aquifer Nodes	VARCAL	WAVE	M

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
HTOL	L	Scalar	Head Tolerance for Matrix Solution of the Unconfined Areal Flow Problem	SMIOIN VARCAL	CONTR3	I,O
HVAR	L M/L**3	Array	Intermediate Values (Head/Conc.) at Aquifer Nodes	VARCAL	WAVE	M
HVTM	L M/L**3	Array	Current Values of Prescribed (Head/Conc.)	SMIOIN HFINTP	BCDATA	I,O
IAQ	--	Scalar	Aquifer Numbering Index	SMIOIN		M
				ASSEMV		O
				BALCHS		
				CPCAL		O
				EBFOR1		M
				EBFPR2		M
				MATMOD		M,O
				VARCAL		
				VELCOM		M
IAQNO	--	Array	Aquifer No. Identification of Various Rectangular Elements	SMIOIN ASSEMV EBFOR1 EBFOR2 MATMOD VELCOM	MDATAQ	M
IAQTYP	--	Array	Aquifer Type Specification	SMIOIN EBFOR1 VARCAL	MDATAQ	I,O
IAREAL	--	Scalar	Areal Modeling Indicator	SMIOIN ASSEMV BALCHS EBFOR1 FILVEL VARCAL VELCOM	CONTR1	I,O
IATP	--	Array	Material Identification for Aquitard Columnb	SMIOIN CPCAL FILPRW MATMOD	MDATAT	M

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
IAXSYM	--	Scalar	Parameter Indicating if AXSYM Used (1=YES, 0=NO)	SMIOIN	CONTR1	I,O
				ANDCAL		
				ASSEMV		
				BALCHS		
				EBFOR1		
				EBFOR2		
				QCAL		
IBSUB	--	Scalar	Matrix Solution Index	CPCAL		
ICALL	--	Scalar	Option Specification Parameter for Matrix Modifications	ASSEMV		O
				MATMOD		
				CPCAL		
				TRIMOD		
ICEND	--	Scalar	Ending Node Number	FIVEIO		I,M,O
				FRVEIO		I,M,O
ICOORD	--	Scalar	Coordinate Generation Index (1 for X-COORD, 2 for Y-COORD)	DXYGEN		
ICOUNT	--	Scalar	Dummy Integer Variable	SMIOIN		M
				ASSEMV		M,O
				BALCHS		
				EBFIND		M
				FILHED		O
				FILPLT		O
				FILPRW		
				FILVEL		O
				FIVEIO		M
				FRVEIO		M
				HFINTP		M
				MATMOD		
				PBC		M
				QCAL		M
IDPCOL	--	Scalar	Aquitard Column Numbers Where Nodal (Head/Conc.) are to be Printed	SMIOIN	PRCNTR	M
				FILPRW		
IDPND	--	Array	Aquifer Node Numbers Where Nodal (Head/Conc.) are to be Printed	SMIOIN	PRCNTR	M
				FILPRW		

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
IDTEMP	--	Array	Temporary Integer Flag Array	ASSEMV PBC	ATEMP	M,O M
IHALFB	--	Scalar	Half Bandwith of Global Matrix	SMIOIN ASSEMV EBFIND MATMOD QCAL SOLVEC SOLVEP VARCAL		M
III	--	Scalar	Unconfined Flow Nonlinear Iteration Index	ASSEMV VARCAL		O
IKALL	--	Scalar	Time Stepping Scheme (0=Central Diff, 1=Backward Diff)	SMIOIN VARCAL	CONTR3	I,O
IMBAL	--	Scalar	Mass Balance Computation Requirement Index	SMIOIN BALCHS FILVEL	CONTR1	
IMODL	--	Scalar	Modeling Type Index (1=Flow, 0=Transport)	SMIOIN ASSEMV BALCHS FILPRW MATMOD QCAL VARCAL	CONTR1	I,O
INDKP	--	Scalar	Node Number of Flux Nodes	SMIOIN QCAL	WAVE2	
INDSTO	--	Array	Nodal Indices of Flux Nodes	BALCHS	WORKS	M,O
IO	--	Scalar	Parameter Controlling Functions of Subroutine (1 for Read, 2 for Write)	FIVEIO FRVEIO		

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
IOBSND	--	Scalar	Observation Node Parameter Specification (1=YES, 0=NO)	SMIOIN	CONTR4	I,O
IOUTLT	--	Scalar	Fluxe Computation Index (1=YES, 2=NO)	SMIOIN	CONTR2	I,O
IPRCHK	--	Scalar	Matrix Computation Print-Check Index (1=YES, 2=NO)	SMIOIN CPCAL EBFOR1 EBFOR2 MATMOD	CONTR4	I,O
IPRCON	--	Scalar	Printout Deletion Index (1=YES, 0=NO)	SMIOIN	CONTR4	I,O
IPRD Requirements	--	Scalar ASSEMV	Printed Output	SMIOIN	CONTR5	I,O
IPROP	REPORT	Array	Material Property Number of the Element	SMIOIN ASSEMV EBFOR1 EBFOR2 MATMOD VARCOM	MDATAQ	O
IRCOUN	--	Array	Recharge Nodal Index Array	SMIOIN BALCHS MATMOD	RCHDAT	M,O
IREPB	--	Scalar	Parameter Indicating if Transient Boundary Condition Date is the same as Preceding Record (1=YES, 0=NO)	SMIOIN RUPDAT		I
IRND	--	Array	Nodal Recharge Index	SMIOIN MATMOD	RCHDAT	M M
IRZKP	--	Array	Zone Numbers of the Recharge Nodes	SMIOIN	RTDATA	I
IRZON	--	Scalar	Recharge Zone Number	SMIOIN		I

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ISLNO	--	Scalar	Aquifer Numbering Index	SOLVEC SOLVEP		
ISTART	--	Array	Starting Node Number of Related Aquifer	ASSEMV BALCHS EBFIND QCAL	ASOLV	M
ISUB	--	Scalar	Matrix Integration Index for Multilayer Aquifer System	ASSEMV VARCAL		
ISWAP	--	Scalar	Parameter Indicating Direction of Sequential Node Numbering	SMIOIN ANDCAL MESHGN		I,O
ITAP10	--	Scalar	Parameter Specifying Which Data is Written to Tape 10 (1 for MESH DATA, 2 for HEAD or CONCENTRATION)	SMIOIN FILPLT		
ITAP6	--	Scalar	Output Control Parameter	SMIOIN FILPRW		
ITAP8	--	Scalar	Parameter-Controlling Functions of Subroutine (1 for READ, 2 for WRITE)	SMIOIN FILHED		
ITAP9	--	Scalar	Input/Output Control Parameter (1=READ, 2=WRITE)	SMIOIN FILVEL		
ITCLIP	--	Scalar	Windowing Node Numbers for Specific Section	SMIOIN	PRCNTR	M
ITDP	--	Array	Parameters Indicating if the Recharge Rate at the Nodes are Time Dependent	SMIOIN RUPDAT	RTDATA	I

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
ITER	--	Scalar	Current Iteration	SMIOIN BALCHS CPCAL EBFOR1 EBFOR2 HFINTP MATMOD VARCAL VELCOM	CONTR2	O
ITRANS	--	Scalar	Simulation Mode (1=TRANSIENT, 0=STEADY-STATE)	SMIOIN	CONTR2	I,O
ITSTF	--	Array	Time Level Counter	SMIOIN HFINTP	BCDATA	M M
ITSTH	--	Array	Time Level Counter	SMIOIN HFINTP	BCDATA	M M
IVECT	--	Array	Temporary Vector for Storing Integer Variable	FILPLT FIVEIO		M I,O
IVRECH	--	Scalar	Recharge of Infiltration Included (1-YES, 0=NO)	SMIOIN ASSEMV BALCHS	CONTR1	I,O
IVSTED Field in Transport	--	Scalar	Steady State Velocity MATMOD (1=YES, 0=NO)	SMIOIN	CONTR4	I,O
IWATP	--	Scalar	Aquifer System Unconfined (1=YES, 0=NO)	SMIOIN ASSEMV BALCHS CPCAL VELCOM	CONTR1	I,O
IXYRED	--	Scalar	Parameter Indicating if Grid Lines are to be Input	SMIOIN MESHGN		I,O O
IZONO	--	Scalar	Material Number Assigned to a Particular Zone of the Aquifer	RUPDAT		I

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
JJJ	--	Scalar	Solving Option (1=MATRIX SOLUTION, 2=BACK SUBSTITUTION)	SOLVEC VARCAL		
JTSRKP	--	Array	Dummy Bookkeeping Array	SMIOIN RUPDAT	RTDATA	M
KKK	--	Scalar	Solving Option (1=COMPLETE MATRIX SOLUTION, 2=BACK SUBSTITUTION)	SOLVEP VARCAL		
LENREC	--	Scalar	Binary Record Length	FILHED		
				FIVEIO		M
				FRVEIO		M
LENV	--	Scalar	Length of Vector	FILHED		M
				FILPLT		M
				FILVEL		M
				FIVEIO		
				FRVEIO		
LV	--	Array	Used In Matrix Bandwidth Computation	EBFIND	ASOLV	M
MM	--	Scalar	Element Number	EBFOR1 EBFOR2		
MXNAQF	--	Scalar	Maximum Number of Aquifers Allowed (Code Limit Parameter)	SMIOIN ASSEMV BALCHS CPCAL EBFOR1 EBFOR2 FILHED FILPLT FILPRW MATMOD VARCAL VELCOM	MDATAQ	
N	--	Scalar	Number of Rows in Tridiagonal Matrix	TRIMOD		

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NAQFR	--	Scalar	Number of Aquifers	SMIOIN ASSEMV BALCHS CPCAL EBFIND VARCAL	CONTR1	I,O
NAQTRD	--	Scalar	Aquitard Separating 2 Aquifers (1=YES, 0=NO)	SMIOIN ASSEMV BALCHS FILHED FILPRW VARCAL	CONTR1	I,O
NB	--	Scalar	Number of Nodes with Prescribed Concentration	ASSEMV BUPDAT PBC SOLVEC SOLVEP	CONTR5	M
NBAND	--	Array	Storage Array Used in Computation of Matrix Bandwidth	ASSEMV BALCHS EBFIND QCAL	ASOLV	M
NBFVAR	--	Scalar	Number of Transient Flux Boundary Conditions	SMIOIN HFINTP PBC	CONTR5	I,O
NBHVAR	--	Scalar	Number of Transient DIRICHLET Boundary Conditions	SMIOIN HFINTP PBC	CONTR5	I,O
NBOUT	--	Scalar	Number of Nodes Where NONZERO Nodal Flux Values are to be Computed	SMIOIN ASSEMV BALCHS FILVEL QCAL	CONTR5	I,O
NBTO	--	Scalar	Number of Steady DIRICHLET Boundary Conditions	SMIOIN BUPDAT HFINTP PBC	CONTR5	I,O

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NCATRD	--	Scalar	Maximum Number of Aquitard Columns	SMIOIN CPCAL	CONTR2	O
NCOL	--	Scalar	Number of Grid Lines Parallel to Y-Axis	MESHGN		M
NCOLS	--	Scalar	Number of Columns in Rectangular Mesh	SMIOIN ANDCAL MESHGN		I,O M
NCOLWN	--	Array	Number of Nodal Columns in the Window	SMIOIN FILPRW	PRCNTR	M
NDFIX	--	Array	Nodal Value Fixing Flag	ASSEMV PBC SOLVEC SOLVEP	ABOUN	M
NDFLUX	--	Scalar	Number of Steady Flux Boundary Conditions	SMIOIN BUPDAT HFINTP PBC	CONTR5	I,O
NDFLX	--	Array	Local Node Number of a Flux Boundary Condition Node	ASSEMV PBC	ABOUN	M
NDFVAR	--	Array	Node Numbers of Time Dependent Flux Boundary Nodes	SMIOIN HFINTP	BCDATA	I,O
NDHVAR	--	Array	Node Numbers of Time Dependent DIRICHLET (Prescribed Head or Conc.)	SMIOIN	BCDATA	
NDOBS	--	Array	Global Sequential Numbers of Observation Nodes	SMIOIN VARCAL	BNDOUT	I,O
NDOUT	--	Array	Global Sequential Node Numbers of the Nodes for Which Nodal Fluid or Solute Flux Values are to be Computed	SMIOIN ASSEMV BALCHS QCAL	BNDOUT	I,O O

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
NDREV	--	Array	Reverse Node Numbering Index	SMIOIN CPCAL	VDISC	M
NE	--	Scalar	Total Number of Elements in the Grid	SMIOIN ANDCAL FILPLT FILVEL MATMOD THUPDT VELCOM	CONTR2	I,O
NEQ	--	Scalar	Number of Algebraic Equations in the Matrix System	SOLVEC VARCAL		M M
NESL	--	Scalar	Number of Elements Per Aquifer	SMIOIN ASSEMV BALCHS EBFIND	CONTR5	M
NITMAX	--	Scalar	Maximum Number of Time Steps	SMIOIN VARCAL	CONTR3	I,O
NMATAQ	--	Array	Number of Materials Associated With the Receptive Aquifer	SMIOIN	MDATAQ	I,O
NN	--	Scalar	Number of Nodes on the Grid Line	DXYGEN SOLVEC		M M
NNDFLX	--	Scalar	Number of Nodal Flux Values in the Current Time Step	ASSEMV PBC	CONTR5	M
NNDSL	--	Scalar	Number of Nodes Per Aquifer	SMIOIN ASSEMV BALCHS CPCAL EBFIND MATMOD SOLVEC SOLVEP VARCAL	CONTR5	M

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NNDWN	--	Array	Number of Nodes in the Current Window Section	SMIOIN FILPRW	PRCNTR	M
NNOBS	--	Scalar	Number of Observation Nodes	SMIOIN VARCAL	CONTR5	I,O
NNP	--	Scalar	Number of Algebraic Equations in the Matrix System	SOLVEP		
NODF	--	Array	Aquifer Node Numbers With Steady-State Flux Boundary Condition	SMIOIN HFINTP PBC	FDATA	I,O M
NODV	--	Array	Aquifer Node Numbers With Steady-State DIRICHLET Boundary Condition	SMIOIN HFINTP PBC	BDATA	I,O M
NOP	--	Array	Element Connection Data for Finite Element Network	SMIOIN ANDCA ASSEMV BALCHS EBFIND EBFOR1 EBFOR2 FILPLT MATMOD MESHGN THUPDT VELCOM	MSHDAT	O M
NOWRIT	--	Scalar	Head Values Written to Tape 8 (1=Yes, 0=No)	SMIOIN	CONTR4	I,O
NP	--	Scalar	Total Number of Nodal Points in the Grid	SMIOIN ANDCAL BALCHS FILHED FILPLT FILVEL MATMOD PBC THUPDT VARCAL VELCOM	CONTR2	I,O

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NPATCO	--	Array	Number of Nodal Points in Each Aquitard Column	SMIOIN CPCAL FILPRW	CONTR2	I,O
NPATD	--	Scalar	Total Number of Nodes in All Aquitards	SMIOIN FILHED	CONTR2	M
NPLOT	--	Scalar	Time and Head Value Written to TAPE 10 (0=No, N=N th)	SMIOIN	CONTR4	I,O
NRCOUN	--	Scalar	Recharge Node Counter	SMIOIN BLCHK MATMOD	CONTR1	M,O
NREC	--	Scalar	Number of Records	FIVEIO FRVEIO		M M
NROW	--	Scalar	Number of Grid Lines Parallel to X-Axis	MESHGN		
NROWS	--	Scalar	Number of Rows in Rectangular Mesh	SMIOIN ANDCAL BALCHS MESHGN		I,O M
NSTEP	--	Scalar	Controls Printout of Computed Values for Nodal points	SMIOIN BALCHS	CONTR4	I,O
NTCLIP	--	Scalar	Number of Time Steps Where Printed Output is Required	SMIOIN	CONTR4	I,O
NTS	--	Scalar	Number of Time Steps	SMIOIN	CONTR2	I,O
NTSNDF	--	Scalar	Number of Control Points on the Flux-vs-Time Graph for Transient Flux Boundary Condition	SMIOIN HFINTP	BCDATA	I

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
NTSNDH	--	Scalar	Number of Control Points on the Graph of Head (or Conc.) vs. Time Graph for Transient Dirichlet Boundary Condition	SMIOIN HFINTP	BCDATA	I
NTSRCH	--	Scalar	Number of Control (Interpolation) Points on the Graph of Recharge Rate vs. Time	SMIOIN RUPDAT		I
NTSRKP	--	Array	Number of Control Interpolation Points for Individual Recharge Zones	SMIOIN RUPDAT	RTDATA	I
NUMT	--	Scalar	Time Step Number	SMIOIN FILPRW		M
NVPR	--	Scalar	Controls Printout of Computed Element Darcy Velocities	SMIOIN VELCOM	CONTR4	I,O
NVREAD	--	Scalar	Velocity Input From Unit Number 9 (1=Yes, 0=No)	SMIOIN	CONTR4	I,O
NVWRIT	--	Scalar	Element Velocities Written to Tape 9 (1=Yes, 0=No)	SMIOIN	CONTR4	I,O
NWINDO	--	Scalar	Number of Output Window Sections in Aquifer Region	SMIOIN FILPRW	CONTR4	I,O
NZONRT	--	Scalar	Number of Zones with Time-Dependent Recharge Rates	Main	CONTR1	I
OUTFL	--	Scalar	Unit Number of Printer Output File	SMIOIN ASSEMV BALCHS CPCAL FILHED FILPLT FILPRW FILVEL QCAL VARCAL VELCOM		O

Table 8-5. SAFTMOD PROGRAM VARIABLES,, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
PROP	REPORT	Array	Material Property of the Porous Matrix	SMIOIN	MDATAQ	O
				ASSEMV		
				EBFOR1		
				EBFOR2		
				VELCOM		
PVAL	L	Array	Temporary Value Storage Array for Head/ Concentration	ASSEMV	ABOUN	
	M/L**3			PBC		M
				SOLVEC		
				SOLVEP		
QNDOUT	L**3/t	Array	Net Values of Prescribed Volumetric Fluid Fluxes at the Nodes	SMIOIN	BNDOUT	I,O
				BALCHS		M
				FILVEL		M
				QCAL		M
QVAL	L**3/t	Array	Storage Array for Flux from Prescribed Boundary Condition During Matrix Assembly and Solution	ASSEMV	ABOUN	
				PBC		
QVALV	L**3/t	Array	Nodal Volumetric Fluid Flux for Steady-State Flux Boundary Condition	SMIOIN	FDATA	I
				HFINTP		M
				PBC		
QVTEMP	L**3/t	Array	Temporary Storage Array for Flux Values During Assembly and Solution of Element Matrix	ASSEMV	ATEMP	O
QVTM	L**3/t	Array	Injected Fluid Volumetric Flux that are Time Dependent (Transpor Simulation Only)	SMIOIN	BCDATA	I,O
				HFINTP		
R1	L**3/t	Array	Integrated Values of Nodal Recharge Fluxes	SMIOIN	WAVE	M,O
				ASSEMV		M
				BALCHS		M
				FILPRW		M
				MATMOD		M
				SOLVEP		M
				VARCAL		M
				VELCOM		M

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
RADS	L	Array	Aquitard Vertical	CPCAL	TRIDIA	M
RCEL	--	Array	Coordinator Aquifer Retardation for each Element in F.E. Network	SMIOIN EBFOR2	RDATA	M
RCHND	--	Array	Nodal Recharge Value Array	SMIOIN	RCHDAT	M
RCHTM	L/t	Array	Recharge Rate Values Corresponding to Control Points on the Graph of Recharge Rate vs. Time	SMIOIN	RTDATA	I
RCHVAL	L/t	Scalar	Steady-State Default Value of the Recharge Rate for the Zone	RUPDAT		I
RCOEF	--	Array	Aquitard Retardation Factor	SMIOIN	RDATA	I,O
RFLUXV	L**3/t	Array	Nodal Recharge Flux Values	SMIOIN ASSEMV BALCHS	RCHDAT	M
ROWA	--	Array	Row Value Storage Array of the Solution Matrix	ASSEMV BALCHS QCAL	WAVE2	M
ROWR	--	Array	Right-Hand Side Row of the Right Solution Matrix	ASSEMV BALCHS QCAL	WAVE2	M
RPCOL	--	Array	Retardation Parameter for Specific Columns of Aquitard	SMIOIN CPCAL	RDATA	M
RTEMP	--	Array	Temporary Storage Array	BALCHS	WORKS	M
S	L M/L**3	Array	Storage of Head or Conc. During Back Substitution	CPCAL TRIMOD	TRIDIA	
SCFX	--	Scalar	Multiplier to Compute Remaining Node Spacings in the X-Direction	SMIOIN MESHGN		I,O

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
SCFY	--	Scalar	Multiplier to Compute Remaining Node Spacings in the Y-Direction	SMIOIN		I,O
				MESHGN		
SS1KP	--	Array	Element Storage Array	BALCHS	ESTORE	
				EBFOR1		M
				EBFOR2		M
SS2KP	--	Array	Element Storage Array	BALCHS	ESTORE	
				EBFOR2		M
TAP10	--	Scalar	File Unit 10	SMIOIN		
				FILPLT		
TAP8	--	Scalar	File Unit 8	SMIOIN		
				FILHED		
TAP9	--	Scalar	File Unit 9	SMIOIN		
				FILVEL		
THEL	L	Array	Saturated Thickness of Element	SMIOIN	ESTORE	I,M
				EBFOR1		
				EBFOR2		
				FILVEL		M
				THUPDT		M
				VELCOM		M,O
THETA	--	Scalar	Time Weighting Factor	SMIOIN	CONTR3	M
				BALCHS		
				CPCAL		
				EBFOR1		O
				EBFOR2		O
				VARCAL		M
THETM1	--	Scalar	THETA-1	BALCHS	CONTR3	
				CPCAL		
				EBFOR1		
				EBFOR2		
				VARCAL		M
THMXND	L	Array	Nodal Value of Aquifer Thickness	SMIOIN	NDSTOR	M
				MATMOD		
				VELCOM		

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
TIMA	t	Scalar	Starting Time of the Simulation	SMIOIN	CONTR3	I,O
TIME	t	Scalar	Time Value	SMIOIN FILPRW		M,O
TIN	t	Scalar	Value of the First Time Step	SMIOIN BALCHS CAPCAL EBFOR1 EBFOR2 FILPRW	CONTR3	I,O M
TMACCU	L	Scalar	Cumulative Fluid Storage	SMIOIN BALCHS	CONTR1	M M,O
TMCLIP	--	Array	Printout Control for Head/Conc.	SMIOIN	PRCNTR	I,O
TMDCAY	M	Array	Total Accumulated Mass Decay	SMIOIN BALCHS	CONTR1	M M
TMHF	t	Array	Time Values to Control Points on Fluid Flux vs. Time Plot	SMIOIN HFINTP	TMDATA	I
TMHV	t	Array	Time Values to Control Points on the Graph of Head (or Conc.) vs. Time	SMIOIN HFINTP	TMDATA	I,O
TMK	t	Scalar	Current Time Value	RUPDAT		M
TMK1	t	Scalar	Preceeding Time Value at the Interpolation Points	RUPDAT		M
TMK2	t	Scalar	Subsequent Time Value at the Interpolation Points	RUPDAT		M
TMRCH	t	Array	Time Values Corresponding to Control Points on the Graph of Recharge Rate vs. Time	SMIOIN RUPDAT	RTDATA	I

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (continued)

Variable	Units	Type	Description	Sub-routine	Common Block	I,M,O
TMVEC	t	Array	Time Values of Time Steps One Through NTS	SMIOIN FILPRW HFINTP	TMDATA	I,M,O
UNIT	--	Scalar	Parameter-Specifying File Unit for Output	FRVEIO FIVEIO		
VABSND	L/t	Array	Absolute Darcy Velocity for Each Node	MATMOD	NDSTOS	M
VALV	L M/L**3	Array	Storage of VAL During Iterative Solution Process	SMIOIN BUPDAT HFINTP PBC	BDATA	I,O M M
VALVO	L M/L**3	Array	Prescribed Value of Head or Conc. for Steady-State Dirichlet Boundary Condition	SMIOIN BUPDAT	BDATA	I,O
VELX	L/t	Array	Element Value of Darcy Velocity in the X-Direction	SMIOIN EBFOR2 FILVEL MATMOD VELCOM	VELEM	I,O M M,O
VELY	L/t	Array	Element Value of Darcy Velocity in the Y-Direction	SMIOIN EBFOR2 FILVEL MATMOD VELCOM	VELEM	I,O M M,O
VTEMP	L**3/t	Array	Temporary Storage of Nodal Fluid Flux Values	ASSEMV PBC	ATEMP	M,O M
XCTR	L	Array	Element Centroidal Value in the X-Direction	SMIOIN ANDCAL EBFOR1 EBFOR2 FILPLT	VELEM	M,O
XFAC	--	Scalar	Multiplier Used to Compute Remaining Nodal Spacing	SMIOIN DXYGEN		

Table 8-5. SAFTMOD PROGRAM VARIABLES, UNITS, LOCATION, AND VARIABLE DESIGNATION (concluded)

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
XFST	--	Scalar	Starting Coordinate Value	DXYGEN		
XLIM	L	Scalar	Length of Domain	DXYGEN		
XLNODE	L	Array	Nodal Length	SMIOIN	NDSTOR	
				ANDCAL		M
				MATMOD		
XO	L	Scalar	Length Along X-Direction	SMIOIN		I,O
				CPCAL		M
				MESHGN		
XS	L	Array	Temporary Storage of X & Y Coordinates of Grid Lines While Being Computed by the Code	ASSEMV	MSHPAR	
				ANDCAL		M
				DXYGEN		M
XW	L	Array	X-Coordinates of Grid Lines One Through NCOLS Read from User File	SMIOIN	MSHPAR	I,O
				ANDCAL		
				DXYGEN		M
				MESHGN		
YCTR	L	Array	Element Centroidal Value in the Y-Direction	SMIOIN	VELEM	M,O
				FILPLT		
YO	L	Scalar	Length Along Y-Direction	SMIOIN		I,O
				MESHGN		
YW	L	Array	Y-Coordinate of Grid Lines One Through NROWS Read from User File	SMIOIN	MSHPAR	I,O
				DXYGEN		M
				MESHGN		
ZBND	L	Array	Zonal Value of Elevation of the Aquifer Base Above the Datum Plane	SMIOIN	NDSTOR	M
				THUPDT		
				VELCOM		
ZI	--	Scalar	Back Substitution Parameter	TRIMOD		M
				CPCAL		
ZIKP	--	Array	Storage of ZI at Aquifer Aquitard Interface	SMIOIN	VDISC	M
				BALCHS		
				CPCAL		M,O
				MATMOD		M

Table 8-6. MONTE-CARLO PROGRAM VARIABLES

Variable	Type	Description	Subroutine
BBT	Double Precision	Correlation matrix for Monte-Carlo inputs.	Main program, READM, INITMC
CORR	Double Precision Array	Array of correlation terms for summary output variables.	Main Program, STSTIS, OUTPUT
DECOM	Integer	Decomposed correlation matrix for Monte-Carlo inputs.	Main Program, INITMC, RANDOM
DIST	Real Array	Array storing empirical distributions.	Main Program, READM, Random
IN2	Integer	Monte-Carlo input file number.	Main Program, READM
IOUT	Integer	Monte-Carlo summary output file unit number.	Main Program, READM, OUTPUT
IOUT2	Integer	Output file unit number for results of each Monte-Carlo run.	Main Program, STATIS
IRUN	Integer	Do loop counter for Monte-Carlo runs.	Main Program, STATIS
IVAR	Integer	Do loop counter for variable number.	Main Program
LARR	Integer Array	Array storing array addresses for random input variables.	Main Program, READM, INITMC
MCMAX	Integer	Maximum possible number of random input variables.	Main Program
MCVAR	Integer	Number of random input variables.	Main Program, READM, INITMC, RANDOM
NCMAX	Integer	Maximum possible number of variables for which cumulative distributions can be plotted.	Main Program
NDAT	Integer Array	Number of values in empirical distributions.	Main Program, READM, RANDOM
NEMP	Integer	Maximum number of empirical distribution value-probability pairs.	Main Program, READM, RANDOM

Table 8-6. MONTE-CARLO PROGRAM VARIABLES (concluded)

Variable	Type	Description	Subroutine
NMAX	Integer	Maximum possible number of variables for which summary statistics can be printed.	Main Program
NRMAX	Integer	Maximum number of Monte-Carlo runs allowed.	Main Program
NRUNS	Integer	Number of Monte-Carlo Runs.	Main Program READM, OUTPUT
NVAR		Number of summary output variables.	Main Program
PNAME	Character Array	Input labels used to flag random input variables.	Main Program, READM, INITMC
RMC	Real Array	Array of randomly-generated numbers.	Main Program, RANDOM
SNAME	Character Array	Input labels used to flag summary output variables	Main Program, READM, OUTPUT
STAT	Double Precision Array	Array of summary statistics for output variables.	Main Program, STSTIS, OUTPUT
VAR	Real Array	Array storing distribution parameters for random input variables.	Main Program, READM, INITMC, RANDOM
XCDF	Real Array	Array storing values of selected variables for plotting cumulative distributions.	Main Program, STATIS, OUTPUT
XMC	Real Array	Array storing values of summary output variables.	Main Program, STATIS

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